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Modeling of eddy characteristic time in LES for calculating turbulent diffusion flame

Mitsuru Yaga, Hajime Endo, Tsuyoshi Yamamoto, Hideyuki Aoki *, Takatoshi Miura

Department of Chemical Engineering, Tohoku University, 07 Aoba, Aramaki, Aoba-ku, Sendai 980-8579, Japan

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Abstract

We have constructed an eddy characteristic time derived from large-scale motion to calculate the combustion reaction rate using a new eddy dissipation concept (EDC) model, and estimated combustion characteristics in the combustor. The calculated temperature and CH_4 mole fraction distribution are in fairly good agreement with the experimental data. However, the calculated CO mole fraction distribution does not agree well with the measured result of CO mole fraction because of using a simple CO reaction mechanism. This study shows that the combustion simulation using LES with EDC model is effective for calculating the characteristics of turbulent diffusion flame. © 2002 Elsevier Science Ltd. All rights reserved.

1. Introduction

In constructing a new combustor, the furnace is usually scaled up in the order of laboratory-, batch-, pilot- and commercial-scale. This method is expensive and time-consuming. We therefore recommend a method using simulations adjusted on a commercial furnace to predict the combustion characteristics. However, experiments are usually considered to be better for this kind of prediction. It is difficult to measure combustion characteristics such as temperature and chemical compounds even in experiment, and the data include unavoidable errors because the combustion characteristics are complicated under high-temperature conditions. Thus, there is a strong need to establish a suitable combustion simulation model. This simulation model is required for (1) scaling up furnace size, (2) developing new combustor for reducing pollutant formation and adjusting various fuel volumes, and (3) determining suitable operating conditions. It is also expected to provide an effective technology for adjusting various parameters in the future. From the viewpoint of energy saving and reducing the volume of discharged environmental pollutants, there has been increasing pressure to control combustion phenomena. We may not be able to confirm computational accuracy, since it is very difficult to obtain a reliable experimental data such as temperature and chemical species distribution in a furnace. Numerical simulation of combustion phenomena is thus very useful technique. Until now, k–ε two-equation turbulence model [1] has been generally used to simulate engineering turbulent phenomena including combustion [2–4]. However, this model is known to have the defect that the approximation deterioates for a nonisotropic field such as that found in a gas turbine combustor. DNS, one of the flow simulation techniques, considers micro-scale eddy motion, however DNS needs too many grids and short time marching to represent micro-scale eddy motion. It is therefore very difficult to apply DNS to a furnace with large spatial scales. Large eddy simulation (LES) [5] is a method of calculating large-scale flow directly and subgrid-scale flow indirectly. A feature of this method is that subgrid-scale flow is modeled by the eddy viscosity concept and viscosity is further modeled on the basis of balance of energy production and dissipation of turbulent flow. This method

* Corresponding author. Tel.: +81-22-217-7251; fax: +81-22-217-6165.

E-mail address: yaga@tranpo.che.tohoku.ac.jp (H. Aoki).

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Nomenclature

A	pre-exponential factor of rate constant ($cm^3\ mol^{-1}\ s^{-1}\ K^{-1}$)
C_S	Smagorinsky constant (dimensionless)
E	activation energy ($J\ mol^{-1}$)
G	filter function (dimensionless)
h	enthalpy ($J\ kg^{-1}$)
m_i	mass fraction for species i (dimensionless)
P	pressure (Pa)
r	radial distance (m)
R	universal constant of gases ($J\ mol^{-1}\ K^{-1}$)
R_{ij}	Reynolds term ($m^2\ s^{-2}$)
R_i	chemical reaction rate ($mol\ m^{-3}\ s^{-1}$)
S_{ij}	strain rate (s^{-1})
S_ϕ	volumetric source term of quantity φ
t	time (s)
T	temperature (K)
u_i	velocity component in i direction ($m\ s^{-1}$)
u	axial velocity ($m\ s^{-1}$)
v	radial velocity ($m\ s^{-1}$)
w	tangential velocity ($m\ s^{-1}$)
x_i	coordinate in i direction (m)
x	axial distance (m)
Δ	filter width (m)
α	stoichiometric oxidant requirement to burn 1 kg of fuel (dimensionless)
δ_{ij}	Kronecker's delta (dimensionless)
ε	eddy dissipation rate ($m^2\ s^{-3}$)
μ	viscosity (Pa s)
ν	kinematic molecular viscosity ($m^2\ s^{-1}$)
ν_t	eddy viscosity ($m^2\ s^{-1}$)
θ	tangential angle (rad)
ρ	density ($kg\ m^{-3}$)
σ_h	Prandtl number (dimensionless)
σ_m	Schmidt number (dimensionless)
τ	eddy characteristic time (s)
Γ_ϕ	diffusion coefficient (dimensionless)
ϕ	generalized variable or equivalence ratio (dimensionless)

Subscripts

Arr	Arrhenius
eff	effective
eddy	eddy mixing
fu	fuel
in	inlet
ox	oxidant

Superscripts

–	spatial average
∼	favre average

thus reduces the number of required grids compared with DNS, and catches instantaneous large-scale eddy motions. For this reason, efforts have been made to apply the LES method to combustion phenomena in recent years [6]. The problem is that there is no confirmed combustion reaction model applied to LES. While the probability density function (PDF) method is often used in LES combustion simulation [7], it takes too long to solve PDF at all cells. We therefore adopt the eddy dissipation concept (EDC) model as a reaction model in this study. When EDC is applied to combustion simulation together with the k–ε two-equation model, it is easy to estimate an eddy characteristic time using time-averaged turbulence energy and eddy dissipation rate. In contrast with the k–ε two-equation model, we cannot easily determine the eddy characteristic time in LES. We thus develop a method for determining an eddy characteristic time to be able to carry out LES combustion simulation using EDC.

2. Simulation method

2.1. Governing equation

All transport equations in this study can be expressed for cylindrical three-dimensional geometry as

$$\frac{\partial}{\partial t}(\rho\phi)+\frac{\partial}{\partial x}(\rho u\phi)+\frac{1}{r}\frac{\partial}{\partial r}(r\rho v\phi)+\frac{1}{r}\frac{\partial}{\partial\theta}(\rho w\phi)=\frac{\partial}{\partial x}\left(\Gamma_\phi\frac{\partial\phi}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\Gamma_\phi\frac{\partial\phi}{\partial r}\right)+\frac{1}{r}\times\frac{\partial}{\partial\theta}\left(\Gamma_\phi\frac{\partial\phi}{\partial\theta}\right)+S_\phi, \quad (1)$$

where ϕ represents the dependent variables which denote the mass (1), momentum (u, v, w), enthalpy (h) and mass fraction (m_i; $i = CH_4$, O_2, CO_2, H_2O, N_2, CO and H_2). Γ_ϕ is the exchange coefficient; S_ϕ is the source term in the gas phase, ρ is the density; and x, r and θ are axial, radial and tangential coordinates, respectively. Density is obtained from equation of state. Overbar means a spatial average. The source terms and exchange coefficients are shown in Table 1. The wall function model [8] is applied to calculate the momentum and energy transport near the wall. Radiative heat transfer is calculated by a 6-flux model [9].

3. Mathematical modeling

LES is a method of solving the spatial-averaged Navier–Stokes equation. In this method, dependent variables are divided into resolved scale and subgrid-

Table 1
Source terms and diffusion coefficients for governing equations

	ϕ	Γ_ϕ	S_ϕ
Mass	1	0	0
Axial momentum	u	μ_{eff}	$\frac{\partial}{\partial x}\left(\mu_{\text{eff}}\frac{\partial u}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{\text{eff}}\frac{\partial v}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial\theta}\left(\mu_{\text{eff}}\frac{\partial w}{\partial x}\right)-\frac{\partial P}{\partial x}$
Radial momentum	v	μ_{eff}	$\frac{\partial}{\partial x}\left(\mu_{\text{eff}}\frac{\partial u}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu_{\text{eff}}\frac{\partial v}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial\theta}\left\{r\mu_{\text{eff}}\frac{\partial}{\partial r}\left(\frac{w}{r}\right)\right\}-2\frac{\mu_{\text{eff}}}{r}\left(\frac{\partial w}{r\partial\theta}+\frac{v}{r}\right)+\frac{\rho w^2}{r}-\frac{\partial P}{\partial r}$
Tangential momentum	w	μ_{eff}	$\frac{\partial}{\partial x}\left(\mu_{\text{eff}}\frac{\partial u}{r\partial\theta}\right)+\frac{\mu_{\text{eff}}}{r}\left\{r\frac{\partial}{\partial r}\left(\frac{w}{r}\right)+\frac{1}{r}\frac{\partial v}{\partial\theta}\right\}+\frac{1}{r}\frac{\partial}{\partial r}\left\{r\mu_{\text{eff}}\left(\frac{1}{r}\frac{\partial v}{\partial\theta}\right)-\frac{w}{r}\right\}+\frac{1}{r}\frac{\partial}{\partial\theta}\left\{\mu_{\text{eff}}\left(\frac{\partial w}{r\partial\theta}+\frac{2v}{r}\right)\right\}-\frac{\rho vw}{r}-\frac{\partial P}{r\partial\theta}$
Mass fraction	m_i	$\frac{\mu_\ell}{\sigma_{\text{m}\ell}}+\frac{\mu_{\text{t}}}{\sigma_{\text{mt}}}$	R_i
Enthalpy	h	$\frac{\mu_\ell}{\sigma_{\text{h}\ell}}+\frac{\mu_{\text{t}}}{\sigma_{\text{ht}}}$	$2a_{\text{R}}(F_x+F_r+F_\theta-3E)$

$$\mu_{\text{t}}=Cs\rho\Delta^2\left\langle 2\left[\left\{\frac{1}{2}\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial x}\right)\right\}^2+\left\{\frac{1}{2}\left(\frac{\partial w}{\partial r}+\frac{\partial u}{r\partial\theta}\right)\right\}^2+\left\{\frac{1}{2}\left(\frac{\partial v}{r\partial\theta}+\frac{\partial w}{\partial r}-\frac{w}{r}\right)\right\}^2\right]+\left(\frac{\partial u}{\partial r}\right)^2+\left(\frac{\partial v}{\partial r}\right)^2+\left(\frac{\partial w}{r\partial\theta}+\frac{v}{r}\right)^2\right\rangle^{1/2}$$

$$\mu_{\text{eff}}=\mu+\mu_{\text{t}}$$

σ_{m}	σ_{h}
0.3	0.3

scale (SGS) by a filtering procedure. This procedure is shown by the following equation:

$$\phi(x_i)=\int\int\int_{i=1}^{3}G_i(x_i,x_i')\phi(x_i')\,\mathrm{d}x_i', \tag{2}$$

where $G_i(x_i,x_i')$ is a filtering function and a dashed value means a sub-grid scale value. The dependent variable can be decomposed as given by the following equation:

$$\phi=\overline{\phi}+\phi'. \tag{3}$$

And the density weighted filter is also used for applying LES to combustion simulation.

After the filtering procedure operates on Navier–Stokes equations, the Reynolds term R_{ij} appears. The Reynolds term is modeled as follows:

$$R_{ij}=\frac{2}{3}\widetilde{u_i'u_j'}\delta_{ij}-2\nu_{\text{t}}\tilde{S}_{ij}, \tag{4}$$

where δ_{ij} is Kronecker's delta, ν_{t} is the turbulent viscosity and S_{ij} is the strain rate. S_{ij} is written in detail as below:

$$S_{xx}=\frac{1}{2}\left(\frac{\partial\tilde{u}}{\partial x}+\frac{\partial\tilde{u}}{\partial x}\right), \tag{5a}$$

$$S_{xr}=S_{rx}=\frac{1}{2}\left(\frac{\partial\tilde{u}}{\partial r}+\frac{\partial\tilde{v}}{\partial x}\right), \tag{5b}$$

$$S_{x\theta}=S_{\theta x}=\frac{1}{2}\left(\frac{1}{r}\frac{\partial\tilde{u}}{\partial\theta}+\frac{\partial\tilde{w}}{\partial x}\right), \tag{5c}$$

$$S_{rr}=\frac{1}{2}\left(\frac{\partial\tilde{v}}{\partial r}+\frac{\partial\tilde{v}}{\partial r}\right), \tag{5d}$$

$$S_{r\theta}=S_{\theta r}=\frac{1}{2}\left(\frac{1}{r}\frac{\partial\tilde{v}}{\partial\theta}+\frac{\partial\tilde{w}}{\partial r}-\frac{\tilde{w}}{r}\right), \tag{5e}$$

$$S_{\theta\theta}=\frac{1}{2}\left(\frac{1}{r}\frac{\partial\tilde{w}}{\partial\theta}+\frac{\tilde{v}}{r}\right). \tag{5f}$$

Viscosity ν_{t} is further modeled as follows:

$$\nu_t=(C_{\text{S}}\Delta)^2|\tilde{S}|, \tag{6}$$

$$|\tilde{S}|=(2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}, \tag{7}$$

where C_{S} represents the Smagorinsky constant and we assume it as 0.2 [10].

3.1. Reaction modeling

We use a three-step global reaction mechanisms to express methane–air combustion reaction as

$$CH_4 + 0.5O_2 \Rightarrow CO + 2H_2 \tag{8}$$

$$CO + 0.5O_2 \Longleftrightarrow CO_2 \tag{9}$$

$$H_2 + 0.5O_2 \Longleftrightarrow H_2O \tag{10}$$

Because the methane–air (oxygen) overall reaction ($CH_4 + 2O_2 \Rightarrow CO_2 + 2H_2O$), often adopted in the turbulent combustion simulation to save calculation time, cannot represent CO and H_2, which are formed in local fuel-rich regions. To consider the interaction between eddy motion and chemical reaction, the EDC model is used to express the reaction rate [11] as

$$R_{\text{eddy}} = 4.0\frac{\overline{\rho}}{\tau}\min\left(\frac{\tilde{m}_{\text{ox}}}{\alpha}, \tilde{m}_{\text{fu}}\right), \tag{11}$$

where α is a stoichiometric oxidant requirement to burn 1 kg of fuel, R_{eddy} is the eddy mixing rate of fuel and oxygen and τ is the eddy characteristic time. The eddy characteristic time τ is estimated by considering the Kolmogorov scale as below:

$$\tau = \left(\frac{\nu}{\varepsilon}\right)^{1/2}, \tag{12}$$

where ε is eddy dissipation rate. From the assumption that turbulence energy generation and dissipation are locally equal (it is the same assumption as Smagorinsky model), eddy dissipation rate is written as follows:

$$\varepsilon = 2\nu_t \tilde{S}_{ij}\tilde{S}_{ij}. \tag{13}$$

Eq. (13) is substituted in Eq. (12). As a result, the eddy characteristic time is finally expressed as

$$\tau = \left(\frac{\nu}{2\nu_t \tilde{S}_{ij}\tilde{S}_{ij}}\right)^{1/2}. \tag{14}$$

Considering both the chemical reaction and the eddy motion, reaction rate is expressed as

$$R_i = -\min(R_{\text{eddy}}, R_{\text{Arr}}), \tag{15}$$

$$R_{\text{Arr}} = A[\text{fuel}]^a[\text{oxygen}]^b \exp\left(\frac{-E}{RT}\right), \tag{16}$$

where A is a pre-exponential factor of rate constant, E is the activation energy, R is a universal constant of gases and T is the temperature. The values of coefficients A, E, a and b are referred from Jones and Lindstedt [12], and Westbrook and Dryer [13].

4. Numerical solution

The SIMPLE algorithm with TDMA [14] is used to solve the partial differential equations shown in Eq. (1). In this simulation, equations of continuity, momentum, enthalpy and gas species mass fractions are discretized in space by a control volume method. Quadratic upstream interpolation is adopted in the convective terms and second-order central difference scheme is adopted in the diffusive terms [15]. The fully implicit scheme is used for time marching and time step is 0.0001 s. A schematic diagram of the computational domain is shown in Fig. 1. The coaxial combustor is 200 mm in internal diameter and 800 mm in length. The inner pipe diameter is ∅5 mm and the annulus pipe diameter is ∅23 mm. A computational grid number in the axial, radial and tangential directions are $120 \times 40 \times 50$, respectively.

5. Experiment

A schematic diagram of the experimental setup is shown in Fig. 2. The combustor is 200 mm in diameter and 800 mm in length. The inner pipe diameter is ∅5 mm and the annulus pipe diameter is ∅23 mm. The experimental conditions are shown in Table 2. Flame temperature is measured with a suction pyrometer probe equipped with an R-type thermocouple. Gases are sucked through a water-cooled sampling probe made of stainless steel. The tip diameter of the gas sampling probe is ∅4.32 mm. Intensive cooling starts at the joint of the probe tip with a water jacket cooling system where chemical reaction halts. Sampling gases are analyzed by a gas chromatograph.

6. Result and discussion

Fig. 3 shows the predicted time mean velocity of the combustion gas flow. The zero-axial-velocity line is plotted in Fig. 3. The strength of the vortex shedding is much weaker with heat release; large-scale eddies are broken up because thermal expansion occurs in the vortex core [16].

Fig. 4 shows the distribution of eddy characteristic time calculated by the present model. The eddy characteristic time in the region where CH_4 and O_2 are mixed is short and LES combustion simulation is expected to

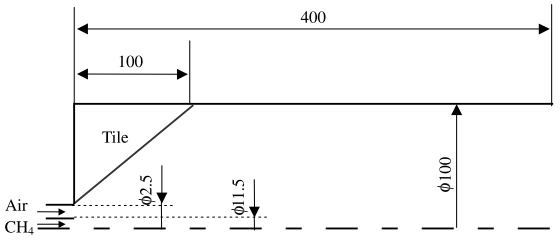

Fig. 1. Schematic diagram of computational domain.

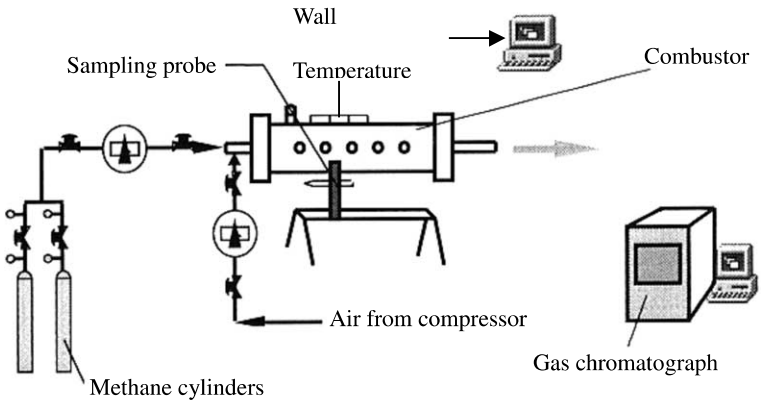

Fig. 2. Schematic diagram of experimental setup.

Table 2
Experimental conditions

ϕ (dimensionless)	1.0
CH_4 ($Nm^3\ h^{-1}$)	0.20
Air ($Nm^3\ h^{-1}$)	1.90
Temperature [K]	293.15
Re_D (dimensionless)	33 228

be carried out under the strict assumption of an eddy dissipation concept model. The combustion reaction occurs when fuel and oxygen are fully mixed in a micro-scale eddy.

Fig. 5 shows the radial distribution of temperature at an equivalence ratio $\phi = 1.0$ at $x = 0.1$ m downstream of the burner. This shows good agreement except at the centerline. The thermocouple system indicates excessive

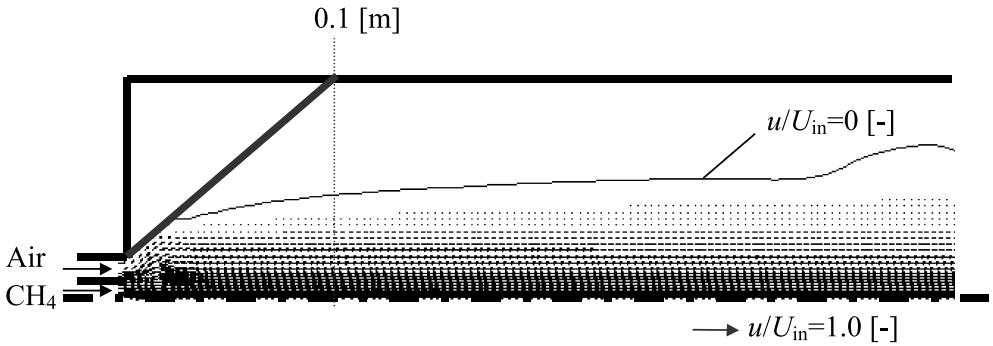

Fig. 3. Predicted time mean velocity vectors in computational domain.

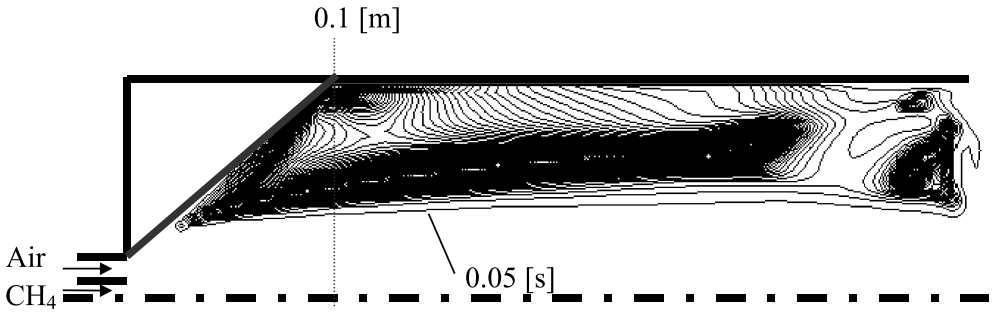

Fig. 4. Calculated instantaneous eddy characteristic time distribution in computational domain.

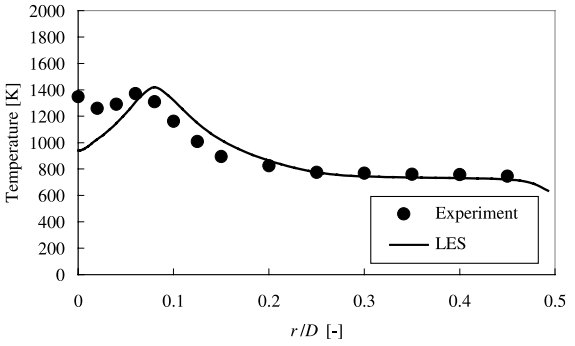

Fig. 5. Radial distribution of temperature at 0.1 m from burner at $\phi = 1.0$.

temperature because the effect of radiation from the suction pyrometer tip is large.

Fig. 6 shows the radial distribution of CH_4 mole fraction at an equivalence ratio $\phi = 1.0$ at $x = 0.1$ m downstream of the burner. This calculation result agrees well with the measured results of CH_4 mole fraction.

Fig. 7 shows the radial distribution of CO mole fraction at an equivalence ratio $\phi = 1.0$ at $x = 0.1$ m downstream of the burner. This calculation result overestimates the experimental result near the centerline. This is because the CO consumption reaction is too simple to correctly estimate the distribution of CO mole fraction.

The selection of a reaction mechanism seriously affects the calculated results of the distribution of chemical species.

Fig. 8 shows the distribution of CH_4 reaction rate calculated by Arrhenius type equation and Fig. 9 shows the distribution of CH_4 reaction rate calculated by eddy dissipation concept model. It is seen that eddy dissipation concept model is dominated near the burner exit and Arrhenius type equation is the main reaction on the flame surface. Considering from these facts, Arrhenius type equation takes an important role on ignition at low temperature field and eddy dissipation concept model affects on mainly preservation of combustion.

Figs. 10 and 11 show the distribution of reaction rate calculated by Arrhenius type equation for H_2 and CO, respectively. From three figures (Figs. 8, 10 and 11), the largest point of CH_4 reaction rate is located around flame bottom surface and the largest H_2 reaction rate is indicated on a slightly downstream of the CH_4 largest

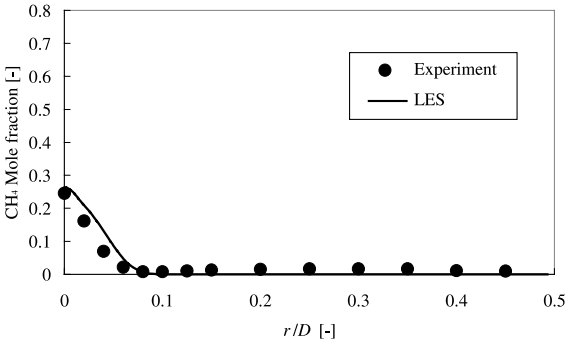

Fig. 6. Radial distribution of CH_4 mole fraction at 0.1 m from burner at $\phi = 1.0$.

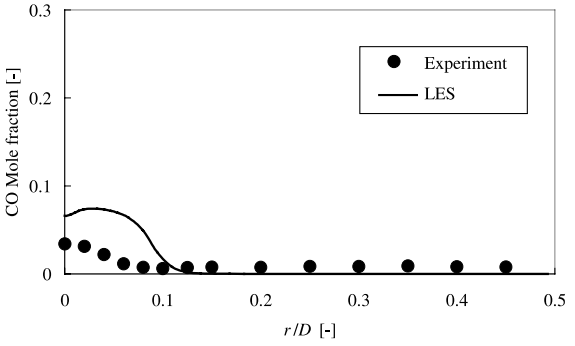

Fig. 7. Radial distribution of CO mole fraction at 0.1 m from burner at $\phi = 1.0$.

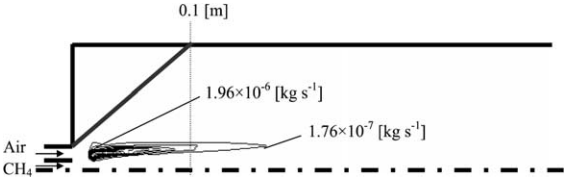

Fig. 8. Calculated CH_4 reaction rate distribution in computational domain by Arrhenius type equation.

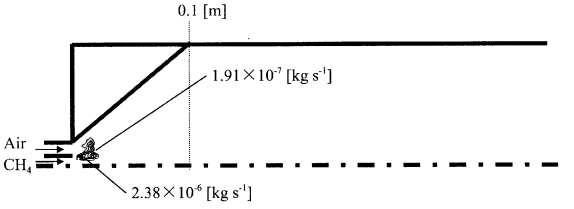

Fig. 9. Calculated CH_4 reaction rate distribution in computational domain by eddy dissipation concept model.

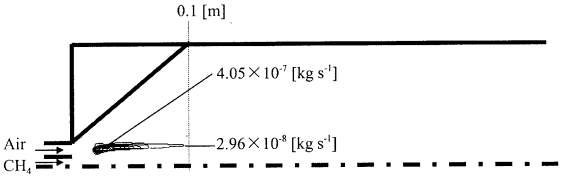

Fig. 10. Calculated H_2 reaction rate distribution in computational domain by Arrhenius type equation.

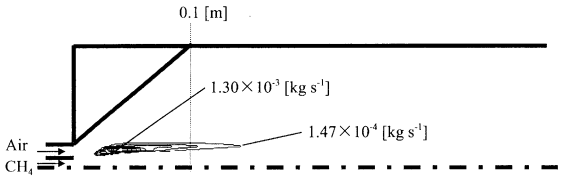

Fig. 11. Calculated CO reaction rate distribution in computational domain by eddy dissipation concept model.

point. Compared with CH_4 and H_2, CO reaction rate indicates larger value on whole flame range. These results show that CH_4 and H_2 combustion are mainly affected by the amount of O_2 and CO combustion is not always so.

7. Conclusion

A three-dimensional large eddy simulation (LES) of a coaxial combustor is carried out. We construct a new eddy characteristic time model derived from a large-scale motion to estimate the combustion reaction rate using an eddy dissipation concept model to save computational time. Estimation of eddy characteristic time considering Kolmogorov scale is effective for determining the subgrid-scale motion of the flame region and the present model more accurately simulates the assumption of the eddy dissipation concept model than a model using time-averaged turbulence energy and eddy dissipation rate. In this study, the calculation results of temperature and CH_4 mole fraction distribution agree well with the measured results. However, the calculated CO mole fraction distribution does not agree well with the measured result of CO mole fraction because of using a simple CO reaction mechanism. If we want to apply LES combustion simulation to engineering applications such as gas turbine combustors, we should thoroughly check the reaction model with the reaction mechanism to determine whether it could be suitable for LES combustion simulation.

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