Validation of a Fractal Dynamic SGS Combustion Model by DNS of Turbulent Premixed Flame in Strong Shear Flow

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ABSTRACT

A fractal dynamic subgrid scale (SGS) combustion model for large eddy simulation (LES) of turbulent premixed combustion which was developed in our previous study (Yoshikawa et al., 2013) is evaluated through static tests on filtered data of direct numerical simulation (DNS) of H_2–air turbulent V-shape premixed flame. The model is based on flamelet concept, fractal characteristics of turbulent premixed flames and scale separation in high Reynolds number turbulence and the accuracy has been demonstrated for freely propagating premixed flame in homogeneous isotropic turbulence (HIT). The results of the static tests validate that the present model has high accuracy and is applicable to conditions where strong mean shear exists and the interaction between flame and turbulence is complex. Furthermore, comparison with some conventional SGS combustion models indicates that the present model has superiority to these models in terms of accuracy.

INTRODUCTION

Large eddy simulation gains more and more attention as a powerful tool for simulating turbulent combustion. Recently, many attempts applying LES to realistic combustion systems have been made (Colin et al., 2000; Pitsch and Duchamp de Lageneste, 2002; Stone and Menon, 2002; Grinstein and Fureby, 2005; Fureby, 2005; Wang and Bai, 2005; Huang and Yang, 2005; Fiorina et al., 2010; Kuenne et al., 2011; Wang et al., 2013). In LES, physical quantities are filtered and divided into the grid scale (GS) and subgrid scale components. Then, large scale unsteady phenomena represented by the GS components are computed, while the contribution of SGS phenomena to those of GS is given by SGS models. Since combustion is intrinsically unsteady, LES is expected to be more accurate than the classical Reynolds Averaged Navier-Stokes (RANS) simulation for numerical simulations of turbulent combustion.

In LES of turbulent combustion, tracking of the flame front is one of the difficulties, since the flame thickness is generally quite thin compared to the LES filter width (Δ), where the filter width should be in the inertial sub-range of turbulent spectrum. For tracking the flame front, G-equation (Kerstein et al., 1988) is frequently used. In the approach, flame front is represented as an infinitely thin scalar iso-surface and its propagation is computed. For extending this approach to LES, G-equation is filtered. Then, a closure model (SGS combustion model) for turbulent burning velocity, S_T, is introduced to solve the filtered G-equation. Since accuracy of LES strongly depends on the SGS model, highly accurate SGS models are required to acquire trustworthy results. However, almost all SGS combustion models used in this approach are those extended from RANS models (Pitsch and Duchamp de Lageneste, 2002; Stone and Menon, 2002; Wang and Bai, 2005; Huang and Yang, 2005) and their accuracy in LES is not assured.

In our previous study (Yoshikawa et al., 2013), a fractal dynamic SGS combustion model based on flamelet concept, fractal characteristics of the flame surface and scale separation in high Reynolds number turbulence for LES of turbulent premixed combustion has been proposed. A series of static tests with DNS data of H_2–air freely propagating flame in HIT has been conducted to evaluate the model, and has demonstrated the accuracy. In practical combustion chambers, however, strong mean shear exists and turbulent combustion characteristics become complicated compared with freely propagating flame in HIT.

In this study, the fractal dynamic SGS combustion model is examined on filtered DNS data of H_2–air turbulent premixed flame with strong mean shear, where V-shape flame configuration (Minamoto et al., 2011) is considered, and the accuracy of the model is evaluated. For comparison, several conventional SGS combustion models are also investigated.

FRACTAL DYNAMIC SGS COMBUSTION MODEL

Detailed derivations of the fractal dynamic SGS combustion model are presented in our previous study (Yoshikawa et al., 2013). The model consists of two parts that represent turbulence and dilatation effects. The former is modelled based on fractal characteristics of the flame surface of turbulent premixed flames and scale separation in high Reynolds number turbulence, while the latter is based on the flamelet concept. Then, the turbulent burning velocity, S_T, is given as the sum of the two parts.

$$\frac{S_T}{S_L} = \frac{A}{\Delta^2} = \frac{A_{\mathrm{turb}}}{\Delta^2} + \frac{A_{\mathrm{div}}}{\Delta^2} \tag{1}$$

where S_L is laminar burning velocity, A denotes the flame surface area, and A_{turb} and A_{div} represent the turbulence and dilatation contributions to the flame surface area, respectively.

It is well known that flame surfaces possess fractal characteristics in flamelet regimes (Shim et al., 2011; Gülder, 2007). Here, it is assumed that the flame surface possesses fractal characteristics in a control volume represented by one grid point of LES. Since the outer-cutoff of the flame front is considered to be equal to the filter width, and the inner-cutoff is scalable by the Kolmogorov length scale (η) (Shim et al., 2011; Tanahashi et al., 2007), the local flame surface area is given as a function of the Kolmogorov length scale and the fractal dimension (D_3):

$$\frac{A}{\Delta^2} = \left(\frac{L_{\mathrm{I.C.}}}{\Delta}\right)^{2-D_3} \approx \left(\frac{\alpha\eta}{\Delta}\right)^{2-D_3} \tag{2}$$

where $L_{\mathrm{I.C.}}$ is inner-cutoff, and α is a scaling factor given by a correlation equation (Shim et al., 2011) between the inner-cutoff and the most expected diameter of the coherent fine scale eddies ($D \approx 8\eta$) and expressed as Eq.(3).

$$\alpha = \frac{L_{\mathrm{I.C.}}}{\eta} = 8\exp\left(C\frac{\delta_{\mathrm{F}}}{D}\right) \tag{3}$$

where C is a model constant set to 6.0 and δ_{F} represents laminar flame thickness based on diffusivity and laminar burning velocity. Then, the Kolmogorov length scale must be modelled using physical quantities of GS.

For modeling the Kolmogorov length scale, scale separation in high Reynolds number turbulence (*i.e.* $l \gg \lambda \gg \eta$, where l and λ are the integral length scale and Taylor microscale, respectively) is assumed. The LES filter width should, originally, be of the order of the integral length scale. Thus, most of the turbulence energy dissipates in SGS ($\varepsilon \approx \varepsilon_{\mathrm{SGS}}$). By assuming the local equilibrium of the energy production, P_{SGS}, and the energy dissipation, $\varepsilon_{\mathrm{SGS}}$, at SGS, applying the Smagorinsky model to the SGS Reynolds stress, and eliminating the dilatation effect from product of the strain rate tensor, S_{ij}, $\varepsilon_{\mathrm{SGS}}$ is expressed as

$$\varepsilon_{\mathrm{SGS}} \approx 2\sqrt{2}\left(C_s\Delta\right)^2\left(\tilde{S}_{ij}\tilde{S}_{ij} - \mathrm{div}\left(\tilde{\boldsymbol{u}}\right)^2\right)^{3/2} \tag{4}$$

where $\tilde{f}$ denotes a Favre averaged quantity of f ($\tilde{f} = \overline{\rho f}/\bar{\rho}$, $\bar{f}$ is a filtered quantity), and C_s is the Smagorinsky constant set to 0.2. In this expression, the strain effect due to turbulence motion is only taken into account, while that caused by dilatation in a flame front is eliminated. By substituting the Kolmogorov length scale calculated with Eq. (4) for Eq. (2), contribution of turbulence to the flame surface area is modelled as

$$\frac{A_{\mathrm{turb}}}{\Delta^2} = \left(\frac{\alpha^4\nu^3}{2\sqrt{2}C_s^2\Delta^6}\right)^{\frac{2-D_3}{4}} \left\{\tilde{S}_{ij}\tilde{S}_{ij} - \mathrm{div}\left(\tilde{\boldsymbol{u}}\right)^2\right\}^{\frac{-3(2-D_3)}{8}} \tag{5}$$

where ν is the kinematic viscosity. Here, D_3 is determined by locally applying the procedure of the fractal dynamic SGS (FDSGS) model (Miyauchi et al., 1994). The model dynamically evaluates D_3 by applying fractal analysis on two levels; the grid and the test filter levels. Detailed descriptions of the model are shown in our previous study (Miyauchi et al., 1994).

The dilatation effect eliminated above is separately modelled based on the flamelet concept. In a laminar flame, dilatation is expressed as du/dx. Assuming that flamelets are distributed on the flame surface, the volume integration of dilation in a control volume represented by a grid point of LES is approximated as

$$\begin{aligned} \frac{A}{\Delta^2}\int_{-\Delta/2}^{\Delta/2}\left(\frac{du}{dx}\right)\Delta^2 dx &\approx A\delta_{\mathrm{L}}\left(\mathrm{div}\left(\boldsymbol{u}\right)_{\mathrm{L}}\right)\Big|_{G=G_0} \\ &\approx \iiint_{\Delta^3}\mathrm{div}\left(\boldsymbol{u}\right)dV \approx \Delta^2\delta_\Delta\left(\mathrm{div}\left(\tilde{\boldsymbol{u}}\right)\right) \end{aligned} \tag{6}$$

where the subscript L represents the values in a laminar flame, δ_{L} is the laminar flame thickness based on the temperature gradient, G is the scalar used in the level-set approach (Kerstein et al., 1988), G_0 is the value of G on the flame surface, and δ_Δ represents a pseudo flame thickness of a filtered laminar flame expressed as Eq (7).

$$\delta_\Delta = \int_{-\Delta/2}^{\Delta/2}\mathrm{div}\left(\tilde{\boldsymbol{u}}\right)_{\mathrm{L}}dx \Big/ \left(\mathrm{div}\left(\tilde{\boldsymbol{u}}\right)_{\mathrm{L}}\right)\Big|_{\tilde{G}=\tilde{G}_0} \tag{7}$$

From Eq. (6), the dilatation effect on the flame surface area is modelled as Eq. (9).

$$\frac{A_{\mathrm{div}}}{\Delta^2} = \frac{\delta_\Delta}{\delta_{\mathrm{L}}} \frac{\mathrm{div}(\tilde{\boldsymbol{u}})}{\left(\mathrm{div}(\boldsymbol{u})_{\mathrm{L}}\right)\big|_{G=G_0}} \tag{8}$$

The actual flame surface area is given as the sum of Eqs. (5) and (8).

DIRECT NUMERICAL SIMULATION OF TURBULENT V-SHAPE PREMIXED FLAME

In this study, the fractal dynamic SGS combustion model is evaluated with DNS data of H_2−air turbulent V-shape premixed flame. Detailed descriptions of DNS are found in our previous paper (Minamoto et al., 2011). Figure 1 shows a schematic of the turbulent V-shape premixed flame simulated in DNS. The turbulent flame is anchored using a hot rod of diameter, $d \approx \delta_{\mathrm{L}}$, and temperature, $T_{\mathrm{rod}} = 2000$ K, which is located at a distance of about 2.5mm from the inflow boundary. The computational domain size, $L_x \times L_y \times L_z$, is $10 \times 5 \times 5$ (in mm). The fluid velocity, $\boldsymbol{U}_{\mathrm{in}}$, at the inlet boundary is specified to be a sum of an average velocity, $\boldsymbol{U}_{\mathrm{av}}$, and a turbulent fluctuation, $\boldsymbol{u}'_{\mathrm{in}}$. The average velocity is $\boldsymbol{U}_{\mathrm{av}} = (U_{\mathrm{av}}, 0, 0)$ and the turbulent velocity fluctuations are obtained from preliminary DNS of incompressible homogeneous isotropic turbulence using spectral methods (Tanahashi et al., 1997). After running the simulation until turbulent and flame are fully developed, the data of the instantaneous filed is extracted and used for static tests of the present model.

Table 1 indicates the numerical condition of the V-shape flame simulated in this study. Here, Re_λ and Re_l are Reynolds numbers based on Taylor micro-scale and integral length scale, respectively, and u'_{rms} represents root mean square of velocity fluctuation at the inlet. As indicated in Fig. 2, the condition locates close to the boundary between the thin reaction zones regime and the corrugated flamelets regime in the turbulent combustion diagram of Peters (2000). The uniform numerical grid of $513 \times 257 \times 257$ is used, which insures that there are at least 20 grid points inside δ_{L}. Also, this grid resolution is sufficient to resolve the boundary layers near the rod and scalar gradients. The governing equations are discretized by fourth-order finite central difference scheme in all directions. The computational boundaries in the inhomogeneous directions, x and y, are specified appropriately to be inflow or outflow boundaries using NSCBC methods (Poinsot and Lele, 1992; Baum et al., 1994) and a periodic boundary condition is used for the homogeneous direction, z. Time integration is implemented by the third-order Runge–Kutta scheme.

EVALUATION OF THE FRACTAL DYNAMIC SGS COMBUSTION MODEL

Static tests on filtered DNS data of turbulent V-shape premixed flame are conducted to investigate the accuracy of the SGS combustion model presented in the previous section. Detailed procedures of static test are presented in our previous study (Yoshikawa et al., 2013). Figure 3 indicates an instantaneous temperature field obtained from DNS on an x-y cross sectional plane. The solid line represents a temperature contour line of 1282 K. Since 1282 K is the temperature that accompanies the maximum heat release rate in a H_2−air laminar flame under the same condition with DNS, the contour surfaces of the temperature are used as representatives of the flame surface in this study. Though the surfaces are wrinkled by turbulence, they remain continuous as it can be expected from the turbulent combustion diagram.

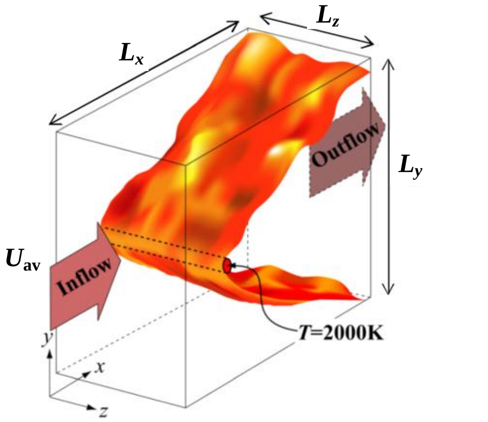

Figure 1. Computational configuration of DNS of turbulent V-shape premixed flame.

Table 1. Numerical condition of DNS of turbulent V-shape premixed flame.

Re_λ	Re_l	η [μm]	l [mm]	u'_{rms} [m/s]
60.8	199.8	15.6	0.793	34.76

U_{av} / S_L	u'_{rms} / S_L	l / δ_{L}	l / δ_{F}
10	3.39	1.69	90.5

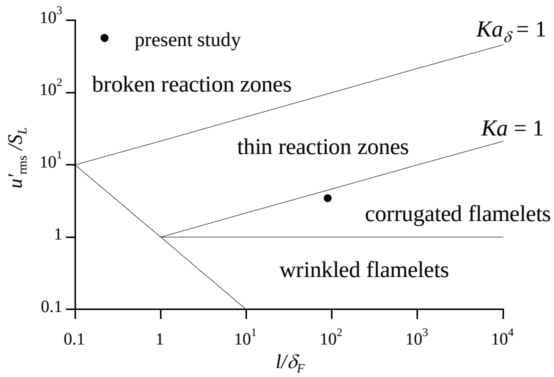

Figure 2. Location of numerical condition of the DNS on the turbulent combustion diagram.

For the static tests of the model, the DNS data are filtered in Favre average manner with a Gaussian or Tophat filter. The filter width, Δ, is set to 20.1η or 40.1 η, which are in the inertial sub-range of turbulent spectrum. The filtered temperature contour surface of 1282 K is then used to define the flame surface in LES. The flame surface is tracked with the G-equation on relatively coarse LES grids of grid size Δ. For extracting LES grid points that track the flame front, the signed distance function from the flame surface is used. This approach is known as the level-set approach and the function is one of the typical definitions of scalar G computed with the G-equation.

If the sign of the calculated signed distance function changes within the filter width from a grid point, and its absolute value at this point is smaller than those at detached points that locate at $\pm\Delta$ in each direction, the point is identified as a tracking point of the LES flame front. Note that LES grids of grid size Δ can be defined in $(\Delta / \Delta_{DNS})^3$ ways depending on the relative position to the DNS grids, where Δ_{DNS} is the DNS grid size. By applying the scheme to all the DNS grid points, all possibilities of LES grid position are covered. In Fig. 4, distribution of flame tracking points identified with Gaussian filter of Δ = 20.1η on a typical cross sectional plane is shown. Black and white lines represent the temperature contour lines of 1282 K of DNS and filtered DNS, respectively. The dark gray zones denote distribution of points that are considered as tracking point of the LES flame front. By applying the model at the flame tracking points, the accuracy of the model is statistically evaluated.

Prior to the present SGS combustion model, several conventional models listed in Tab. 2 are examined for comparison. The models of Colin et al. (2000) and Charlette et al. (2002) are proposed in the thickened flame context. The thickening factor F is set to 1.0 for the test. The velocity fluctuations at the filter width scale, u'_Δ, required by each model are calculated from the DNS data. In Fig. 5, the joint probability density functions (JPDFs) of the flame surface area obtained from the DNS data and predicted with the conventional models are shown. The horizontal and vertical axes are for the DNS data and the model predictions, respectively. The black line in each figure represents the points where the model prediction coincides with the DNS data. The probability difference between two neighboring contour lines is 2.0. These results are obtained with Gaussian filter of Δ = 20.1η. With the model of Charlette et al., a term in a square root in the fitting function becomes negative and the model is not applicable. The flame surface areas predicted by the models of Colin et al. and Flohr et al. (2000) are almost constant values and considerably smaller than the DNS data. Though those by the model of Pitsch et al. (2002) are closer to the DNS data, they are still smaller. Since it is observed that the conventional SGS combustion models underestimate the flame surface area, these models are expected to give significantly smaller turbulent burning velocity than the DNS values under the conditions applied in this study.

In the same manner, the fractal dynamic SGS combustion model is tested. The fractal dimension of the flame surface required by the model is determined with the procedure of FDSGS model (Miyauchi et al., 1994). The test-filter width used in FDSGS model is set to $\hat{\Delta} = 2\Delta$. The procedure of FDSGS model is locally applied in cubic control volumes (CVs) centered by a target grid point. Two CV sizes are tested; 4Δ and 8Δ in edge length. To prevent unphysical values of the fractal dimension, the dimension is clipped at 2.0 and 3.0, so that it remains in this range. JPDFs of the local flame surface area obtained from the DNS data and predicted with the

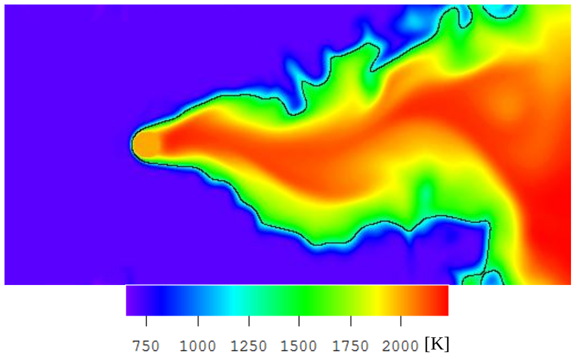

Figure 3. An instantaneous temperature field of DNS on an *x-y* cross sectional plane.

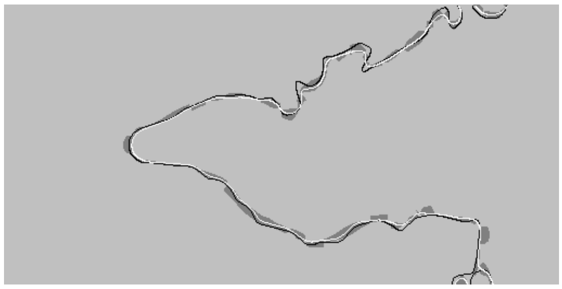

Figure 4. Flame front identification in LES. Gaussian filter with Δ = 20.1η is used.

Table 2. Conventional SGS combustion models.

	Function and parameters for the wrinkling factor
Colin et al. (2000)	$\Xi = 1+\beta \frac{2\ln(2)}{3c_{ms}\left(Re_t^{1/2}-1\right)}\Gamma\left(\frac{\Delta}{\delta_F},\frac{u'_\Delta}{S_L}\right)\frac{u'_\Delta}{S_L}$ $\beta = 1$
Charlette et al. (2002)	$\Xi = \left(1+\min\left[\frac{\Delta}{\delta_F},\Gamma\left(\frac{\Delta}{\delta_F},\frac{u'_\Delta}{S_L},Re_\Delta\right)\frac{u'_\Delta}{S_L}\right]\right)^{\beta}$ $\beta = 0.5$
Flohr and Pitsch (2000)	$\Xi = 1+a(Re_\Delta Pr)^{1/2}Da_\Delta^{-1/4}$ $a = 0.52$
Pitsch and Duchamp de Lageneste (2002)	$\Xi = 1+\frac{u'_\Delta}{S_L}b_3\left[(Da_\Delta/Sc_\Delta)/\left(1+\frac{b_3^2}{b_1^2 Sc_\Delta}Da_\Delta\right)\right]^{1/2}$ $b_1 = 2;\quad b_3 = 1$

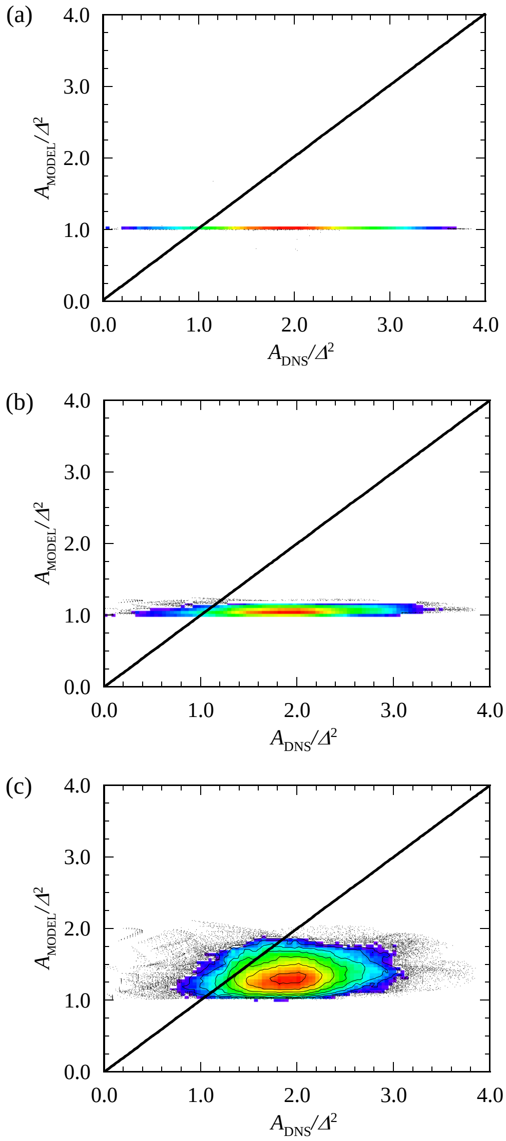

Figure 5. Joint probability density functions of flame surface area obtained from the DNS data and prediction of the conventional SGS combustion models: Colin et al. (2000) (a), Flohr et al. (2000) (b), and Pitsch et al. (2002) (c). Gaussian filter with $\Delta = 20.1\eta$ is used.

fractal dynamic SGS combustion model are indicated in Fig. 6. Figures 6(a), 6(b), and 6(d) are obtained with Gaussian filter, while Fig. 6(c) is with Tophat filter. These results are obtained with $\Delta = 20.1\eta$ (Figs. 6(a), 6(c), and 6(d)) or $\Delta = 40.1\eta$ (Fig. 6(b)), and CV size $(4\Delta)^3$ (Figs.6(a), 6(b), and 6(c)) or CV size $(8\Delta)^3$ (Fig. 6(d)) is applied. As it is clearly shown, the positions of the most expected value of JPDFs are quite close to the black line, being independent of the filter width, filter type and CV size. From these results, it is validated that the present model has high accuracy to predict flame surface area for the turbulent premixed flame with strong mean shear. The predicted values in the results scatter because of the fact that Smagorinsky coefficient is constant and several

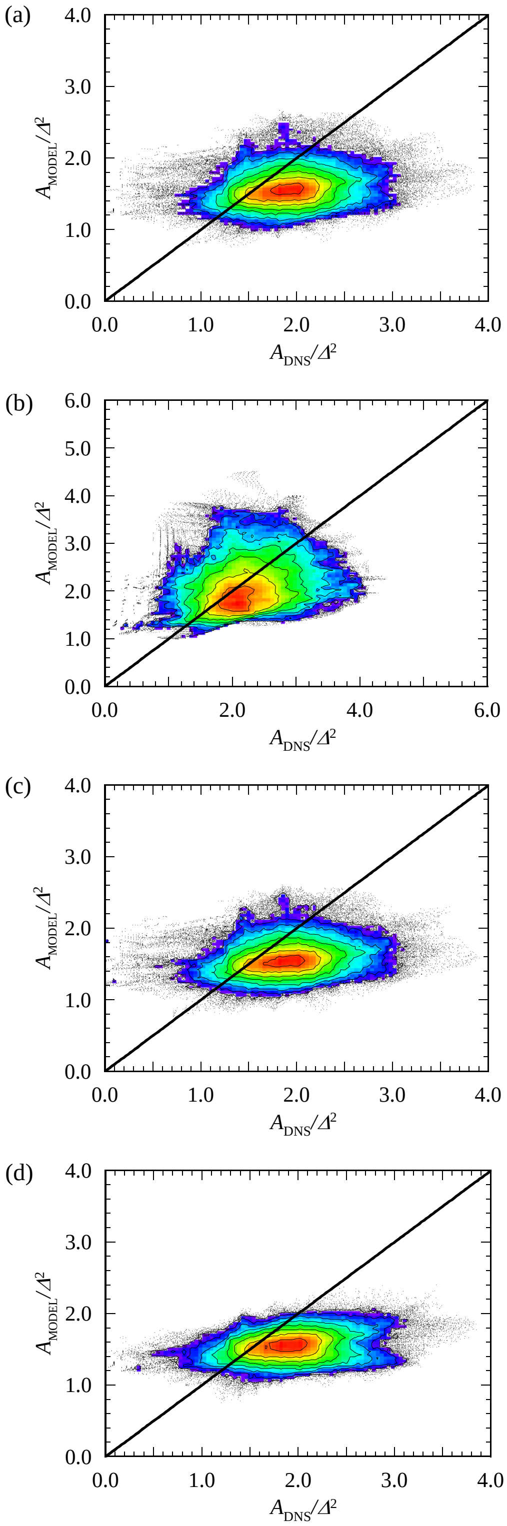

Figure 6. Joint probability density functions of flame surface area of the DNS data and prediction of the fractal dynamic SGS combustion model. (a): Gaussian filter of $\Delta = 20.1\eta$, and CV size $= (4\Delta)^3$. (b): Gaussian filter of $\Delta = 40.1\eta$, and CV size $= (4\Delta)^3$. (c): Tophat filter of $\Delta = 20.1\eta$, and CV size $= (4\Delta)^3$. (d): Gaussian filter of $\Delta = 20.1\eta$, and CV size $= (8\Delta)^3$.

expressions are statically obtained. To improve the precision, it may be good choice that Smagorinsky model which dynamically determine the coefficient is applied. Finally, comparison of the results with those of the conventional models indicates that the fractal dynamic SGS combustion model is superior to the conventional models under the condition applied in this study.

CONCLUSION

In this study, a fractal dynamic SGS combustion model for LES of turbulent premixed combustion which was developed based on fractal characteristics of turbulent premixed flames and scale separation in high Reynolds number turbulence by introducing the determination procedure of the fractal dimension of the FDSGS model has been investigated through static tests on filtered DNS data of turbulent V-shape premixed flame where strong mean shear exists.

Static tests demonstrate the accuracy of the present model for the turbulent premixed flame with strong mean shear. The model is, thus, expected to be fully applicable to flames in practical configurations which are seen in realistic combustion systems. In addition, the results of the tests show that the present SGS combustion model is superior to the conventional models in terms of accuracy at least under the condition applied in this study.

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