FINE SCALE STRUCTURE OF H_2-AIR TURBULENT PREMIXED FLAMES

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ABSTRACT

Direct numerical simulation of H_2-air turbulent premixed flame propagating in three-dimensional homogeneous isotropic turbulence is conducted to investigate fine scale structure of turbulent premixed flames. Detailed kinetic mechanism including 12 reactive species and 27 elementary reactions is used to represent the H_2-O_2 reaction in turbulence. The fine scale structure of turbulent premixed flames is significantly affected by the coherent fine scale eddies in turbulence. The relatively strong coherent fine scale eddies can survive behind the flame front and they are perpendicular to the flame front where heat release rate increases. Direction of the coherent fine scale eddies near the flame front tends to be parallel to the flame front and enhance the chemical reaction. In this case, the distributions of high heat release rate show tube-like structure similar to the coherent fine scale eddies in turbulence. The probability density function (pdf) of local heat release rate is nearly Gaussian with a peak at maximum heat release rate of a laminar flame. The pdf of the curvature of flame front is far from Gaussian and shows exponential tails for large curvature. Most of flame elements are stretched by turbulent motion in the tangential directions. Strong correlation exists between local heat release rate and curvature of flame front. The flame elements convex toward the burnt side with large curvature tend to have high heat release rate. The correlation between local heat release rate and tangential strain rate also exist, while this is not so strong.

INTRODUCTION

Turbulent premixed flames are frequently observed in many engineering applications such as IC engines and gas turbines. However, complicated interactions between chemical reaction and turbulence lead to difficulties in understanding the detailed structure of the turbulent premixed flames. Recent developments of computer technology proved a new tool for the turbulence researches: direct numerical simulation (DNS). DNS of turbulence has succeeded in developments of turbulence models and understanding of the physics of turbulence.

Similar approaches have been applied to the turbulent combustion from a viewpoint of extension of fluid dynamics (Give, 1989). Baum *et al.* (1994a) have conducted direct numerical simulations of H_2-O_2 turbulent premixed flames with complex chemistry and clarified the propagation mechanism in two-dimensional turbulence and characteristics of flamelets in a wide range of equivalent ratio. Effects of strain rate and curvature of the flame fronts in methane-air turbulent premixed flames have been investigated using the results of DNS of methane-air turbulent premixed flames with four-step reduced kinetic mechanism by Echekki and Chen (1996). They have also reported the formation of unburned pocket in turbulent methane-air flames and its dynamics by using DNS data with detailed kinetic mechanism which includes C_1 chemistry (Chen *et al.*, 1998). Miyauchi *et al.* (1997) have conducted DNS of H_2-air turbulent premixed flames and discussed the local flame structure, fractal characteristics of flame surfaces and effects of equivalent ratio etc. Resent progresses in these researches of the turbulent premixed flames by DNS are reviewed by Poinsot *et al.* (1996). By using detailed kinetic mechanism, the mechanism of local extinction and NO_x formations in turbulent methane-air premixed flames are investigated by Tanahashi *et al.* (1999a).

These previous DNS of turbulent premixed flames gave a lot of information about the premixed flames in turbulence,

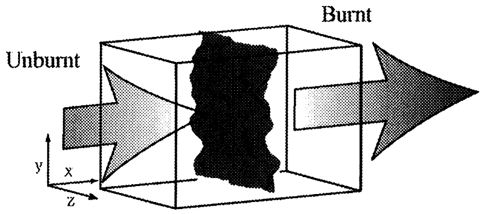

Figure 1. Geometry of flow field.

while all of the previous studies were restricted to 2D calculations due to the limitation of computer resources. Three-dimensional DNS is required to understand the fine scale structure of turbulent premixed flames.

Our resent studies on fine scale structure of turbulence (Tanahashi *et al.*, 1997a: 1997b) show that turbulence consists of coherent tube-like eddies. Mean diameter of those eddies is about 10 times of Kolmogorov micro scale and maximum azimuthal velocity is about a half of r. m. s. velocity fluctuation. As the coherent fine scale eddies of turbulence show strong swirling motion, the interaction between flame and the coherent fine scale eddies should determine the fine scale structure of turbulent premixed flames. In this study, DNS of H_2-air turbulent premixed flames propagating in three-dimensional homogeneous isotropic turbulence are conducted to investigate fine scale structure of turbulent premixed flames.

DNS OF H_2-AIR TURBULENT PREMIXED FLAMES

In this study, we assumed that the external forces, Soret effect, Dufour effect, pressure gradient diffusion, bulk viscosity and radiative heat transfer can be negligible. Details of the governing equations are shown by Miyauchi *et al.* (1996). The viscosity, the thermal conductivity and the diffusion coefficients are calculated by CHEMKIN packages (Kee *et al.*, 1986: 1989), where original programs are modified to be fully vectorized and parallelized. Detailed kinetic mechanism (Gutheil *et al.*, 1993) which includes 27 elementary reactions and 12 reactive species: H_2, O_2, H_2O, O, H, OH, HO_2, H_2O_2, N_2, N, NO_2 and NO is used to represent H_2-air combustion in turbulence.

Inflow boundary condition for chemical species is set equal to H_2-air mixture with $\phi = 1.0$ at 0.1MPa and 700K. Figure 1 shows the schematics of the flow field used in this study. Periodic boundary conditions are applied in the y and z directions and NSCBC (Poinsot and Lele, 1992: Baum *et al.*, 1994b) is used in the x direction. A spectral method is used to discretize the governing equations in the y and z directions and a fourth order central finite difference scheme is used in the x direction. Aliasing errors from nonlinear terms in the y and z directions are fully removed by 3/2 rule. Time integration is conducted by the third order Runge-Kutta scheme.

Inflow boundary condition for the velocity field is given as $u_{in}(y, z, t) = S_L + u'(y, z, t)$, where $u'(y, z, t)$ is a fully developed three-dimensional homogeneous isotropic turbulence and S_L is a laminar burning velocity that is deter-

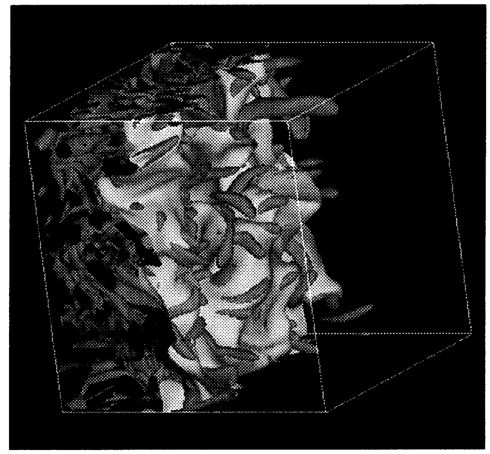

Figure 2. Contour surfaces of second invariant and density (dark gray: Q^+=0.003, gray: $(\rho-\rho_b)/(\rho_u-\rho_b)$= 0.50).

mined by a preliminary one-dimensional flame calculation. The turbulence at the inflow boundary is also obtained by the preliminary calculation of homogeneous isotropic turbulence with a spectral method (Tanahashi *et al.*, 1997a). The calculation of turbulence was conducted with periodic boundary conditions. Reynolds number based on Taylor micro scale is about 37.9. The result at 1 eddy turn over time was converted to the inflow boundary condition by using Taylor's hypothesis and a phase shift technique (Miyauchi *et al.*, 1997: Tanahashi *et al.*, 1998a).

The structure of turbulent premixed flames depends on turbulent intensity and characteristic length scale of turbulence. These effects have been classified by two parameters which are u'/S_L and l/δ_L. Here, l is integral length scale of turbulence and δ_L is a laminar flame thickness. In this study, DNS was conducted for u'/S_L =3.0 and l/δ_L = 1.74. The computational domain is selected to be 0.5cm × 0.5cm × 0.5cm and 257× 128 ×128 grid points are used. This DNS is conducted in 64PE mode of SR2201 massive parallel processors with 5.8 GB total memories and 2000 CPU hours/PE.

FINE SCALE STRUCTURE OF H_2-AIR TURBULENT PREMIXED FLAMES

The coherent fine scale eddies and local flame structure

Our recent studies on the fine scale structure of turbulence (Tanahashi *et al.*, 1997a: 1997b, 1999b) have shown that turbulence has universal fine scale structure which is composed of coherent tube-like eddies. Figure 2 shows the contour surfaces of second invariant of the velocity gradient tensor and density. The second invariant of the velocity gradient tensor is defined as follows:

$$Q = \frac{1}{2}(W_{ij}W_{ij} - S_{ij}S_{ij}), \tag{1}$$

where S_{ij} and W_{ij} denotes symmetric and asymmetric part of the velocity gradient tensor, respectively. The second inva-

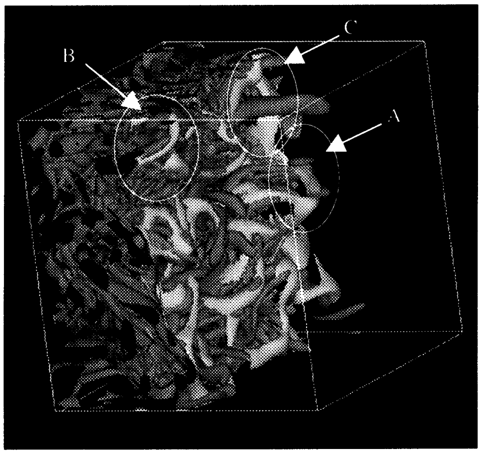

Figure 3. Contour surfaces of second invariant and heat release rate (dark gray: Q^+=0.003, gray: ΔH^* = 1.025).

riant is normalized by Kolmogorov micro scale and u' of unburnt side. The contour levels in Fig. 2 are Q^+ = 0.003 and $(\rho-\rho_b)/(\rho_u-\rho_b)$ = 0.50, where ρ_u and ρ_b denote density in unburnt and burnt side. It was reported by Tanahashi *et al.* (1997a, 1997b) that the coherent fine scale structure of turbulence is well represented by the positive second invariant region in turbulence. Coherent fine scale eddies in homogeneous isotropic turbulence are distributed randomly in space, while those near the flame fronts decays in the flame due to the increase of the viscosity and expansion of fluid. The large modification of the density surfaces can be observed near the relatively strong coherent fine scale eddies in the flame front. The coherent fine scale eddies which are surviving even behind the flame front seem to be perpendicular to the flame front. But the direction of many eddies at the flame front tends to be parallel to the flame front.

Contour surfaces of heat release rate are shown in Fig. 3 with those of second invariant. The local heat release rate is normalized by the maximum heat release rate of a laminar flame (ΔH_L). Hereafter, * denotes the normalization by flame thickness, burning velocity and maximum heat release rate of a laminar flame. The contour level is selected to be 1.025 time of ΔH_L. The maximum heat release rate of this turbulent premixed flame is about $1.2\Delta H_L$. Figure 3 shows that distribution of heat release rate is highly localized by the turbulence-flame interaction. The regions of high heat release rate are observed near the coherent fine scale eddies and are convex toward the burnt side (see a white circle A). Several regions with high heat release rate show tube-like structure and coincide with the coherent fine scale eddies, where a typical regime is denoted by the circle B. Even though the tube-like coherent fine scale eddies exist near the flame, regions with relatively low heat release rate are also observed, which is shown by the circle C. The difference in effects of the coherent fine scale eddies on the local flame structure is caused by the three-dimensionality of the coherent fine scale eddy, which is discussed in Tanahashi *et al.* (1999c).

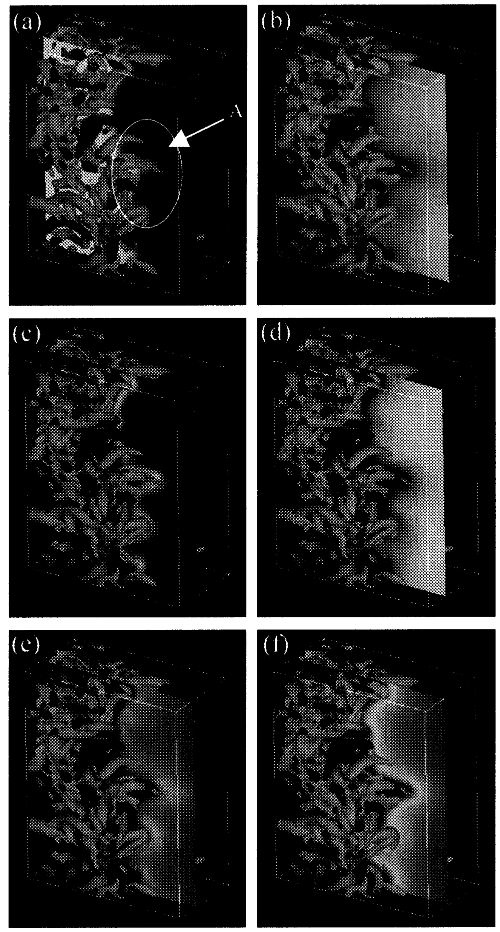

Figure 4. Typical fine scale structure in H_2-air turbulent premixed flames. (a): density, (b): temperature, (c): heat release rate, (d): OH mass fraction, (e): O mass fraction and (f) H mass fraction. Contour surfaces represent the second invariant with Q^+=0.0025.

Figure 4 shows distributions of density, temperature, heat release rate and mass fractions of several species on the typical *x-y* section through A region in Fig. 3. Contour surfaces of second invariant (Q^+=0.0025) are drawn in Fig. 3 to show the relation between local flame structure and coherent fine scale eddies. In the unburnt side of the flame convex toward the burnt side, coherent fine scale eddies perpendicular to the flame front exist. In these regions, heat release rates become high. In our previous studies for turbulent H_2-air premixed flames propagating in two-dimensional homogeneous turbulence (Miyauchi *et al.*, 1997: Tanahashi *et al.*, 1998a: 1998b), it has shown that the modification of the local flame structure is caused by the difference of molecular diffusion coefficients of H_2 and O_2, and that these effects are reflected in the distributions of O and H atoms. OH and H mass fractions seems to be uniform along to the flame front (Fig. 4(d) and (f)), while O

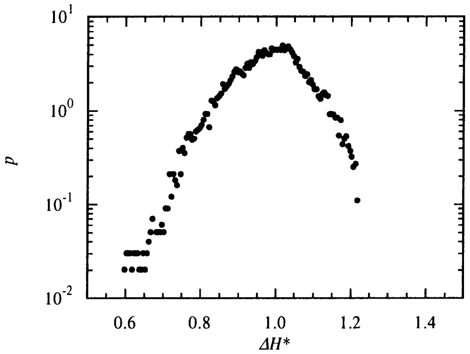

Figure 5. Probability density function of local heat release rate in turbulent premixed flame normalized by maximum heat release rate in a laminar premixed flame.

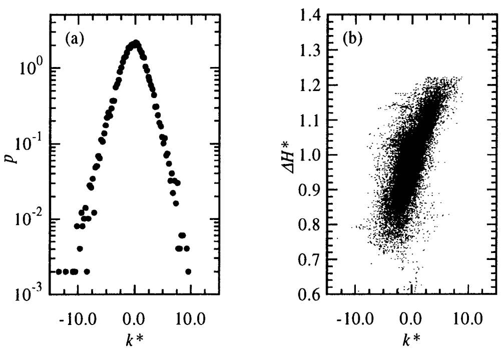

Figure 6. Probability density function of curvature of flame front (a) and scatter plots of the curvature and local heat release rate (b).

mass fraction changes significantly as shown in Fig. 4(e). The distribution of O mass fraction coincides with that of heat release rate in Fig. 4(c). These results are similar to the results obtained in two-dimensional cases reported by Miyauchi *et al.* (1997) and Tanahashi *et al.* (1998a, 1998b).

Statistics of local flame elements in turbulence

In this section, statistical properties of local flame elements are discussed. In this study, the flame fronts ζ are defined as follows;

$$\zeta = \left(\frac{\partial T}{\partial \boldsymbol{n}}\right)_{\max}, \tag{2}$$

where $\boldsymbol{n}$ is a unit vector normal to temperature gradient. Figure 5 shows probability density function (pdf) of maximum heat release rate of a local flame element in three-dimensional turbulence. The pdf of the local heat release rate shows a peak at that of a laminar flame. Due to the turbulence-flame interaction, local heat release rates of flame elements in turbulence are fluctuating. The profile of the pdf seems to be symmetric. The maximum heat release rate reaches to $1.2\Delta H_L$ and the minimum one decreases to $0.6\Delta H_L$. Note that no local extinction can be observed in the present results even if the local heat release rate becomes

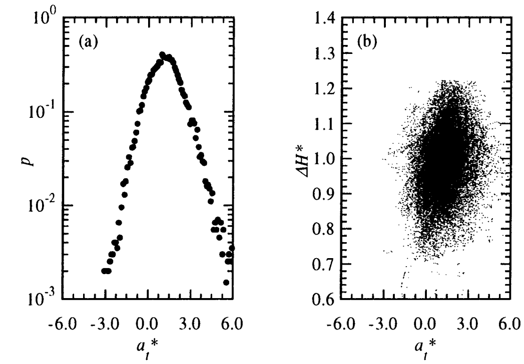

Figure 7. Probability density function of tangential strain rate at flame front (a) and scatter plots of the tangential strain rate and local heat release rate (b).

relatively small.

In the turbulent combustion models, curvature of flame fronts and tangential strain rate on the flame surfaces are important parameters to represent the local flame structure. Figure 6 shows pdf of the curvature and relation between the curvature and the local heat release rate. The curvature is defined as follows:

$$k = \frac{1}{R_1} + \frac{1}{R_2}, \tag{3}$$

where R_1 and R_2 denotes two curvature radius on the flame surface. The flame elements convex toward the burnt side have positive values and the curvature is normalized by the laminar flame thickness. The pdf of curvatures shows nearly symmetrical distribution around $k^* = 0.0$. The profile is far from the Gaussian distribution and shows exponential tails for large $|k^*|$. Figure 6(b) suggests that local heat release rates in turbulence are well correlated with the curvature of the flame front and increase linearly with the increase of k^*. Flame elements convex toward the burnt side show higher heat release rate, which coincides with the observation in Fig. 3.

In Fig. 7(a), pdf of strain rate tangential to the flame front are shown. The tangential strain rate at the flame front are defined as follows (Candel and Poinsot, 1990):

$$a_t = \boldsymbol{t}_1\boldsymbol{t}_1 : \nabla\boldsymbol{u} + \boldsymbol{t}_2\boldsymbol{t}_2 : \nabla\boldsymbol{u}, \tag{4}$$

where $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$ represent unit vectors tangential to the flame front and are satisfying a relation of $\boldsymbol{t}_1 \cdot \boldsymbol{t}_2 = 0$. Positive tangential strain represents the stretched flame element and negative strain does compressed one. The pdf of tangential strain rate shows a peak at a positive value: $a_t^* = 1.0$ and symmetrical distribution, which means that most of flame elements is stretched by the turbulent motion. The pervious results of two-dimensional DNS (Miyauchi *et al.*, 1997: Tanahashi *et al.*, 1998a: 1998b) have shown that tangential strain rate is also correlated with the local heat release rate. Figure 7(b) shows the relation between the tangential strain rate and local heat release rate. The local heat release rates are also correlated with tangential strain rate at the flame front, while the correlation is weaker than

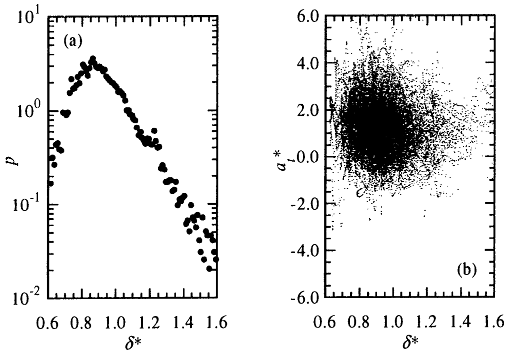

Figure 8. Probability density function of local flame thickness (a) and scatter plots of the flame thickness and the tangential strain rate (b).

that with curvature shown in Fig. 6(b). The heat release rate tends to increase with the increase of the tangential strain rate.

Figure 8(a) shows pdf of local flame thickness defined as:

$$\delta = \frac{T_b - T_u}{(\partial T / \partial n)_{\max}}, \quad (5)$$

where T_u and T_b denote temperature in the unburnt and burnt side. Most expectable flame thickness is about 0.9 δ_L, which means that mean flame thickness becomes thinner than the corresponding laminar flame thickness. The scatter plots between flame thickness and tangential strain rate are presented in Fig. 8(b). In general, it is considered that a stretched flame becomes thinner. Figure 8(b) shows this tendency, while the correlation between them is quite weak.

As shown in the previous section, coherent fine scale eddies of turbulence have significant effects on the local flame structure. Figure 9 shows conditional pdfs of the characteristic properties of the flame element. The pdfs are constructed by conditioning with the sign of the second invariant at the flame front. From the definition in Eq. (1), the rotation rate ($W_{ij}W_{ij}$) is exceeding the strain rate ($S_{ij}S_{ij}$) in the regime with $Q > 0$. Those regions with $Q > 0$ correspond to the coherent fine scale eddies of turbulence. In the regions with $Q < 0$, energy dissipation is dominant.

Conditional pdfs of local heat release rate in Fig. 9(a) show the different distribution for flame element with $Q < 0$ and $Q > 0$. The peak of the pdf is smaller than ΔH_L for $Q < 0$ and greater than ΔH_L for $Q > 0$. These results suggest that rotation-dominant regions tend to enhance heat release rate and the strain-dominant regions tend to suppress heat release rate. The conditional pdfs of the curvature of the flame front show that a lot of flame elements convex toward the burnt side have positive second invariant. This result coincides with the visualizations of flow fields which are presented in the previous section. Compared with heat release rate and curvature, relatively large difference can be observed in conditional pdfs of the tangential strain rate at the flame front. The shape of the pdf with $Q > 0$ is sharper

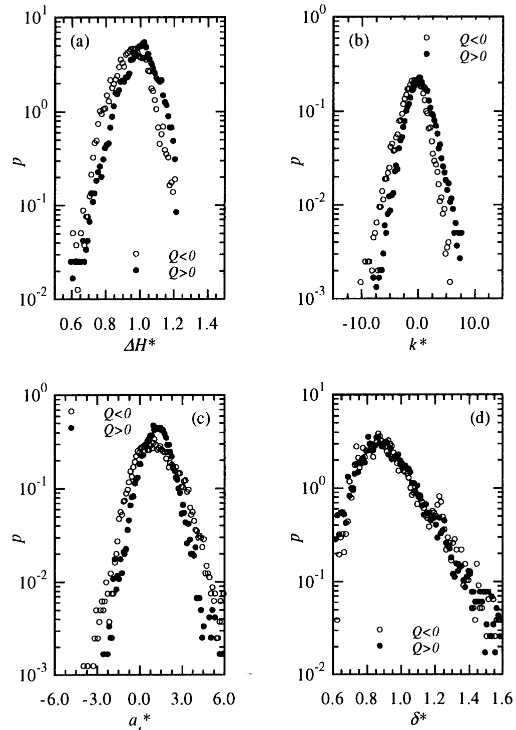

Figure 9. Probability density functions of local heat release rate (a), curvature (b), tangential strain rate (c) and local flame thickness (d) conditioned with sign of second invariant at the flame front.

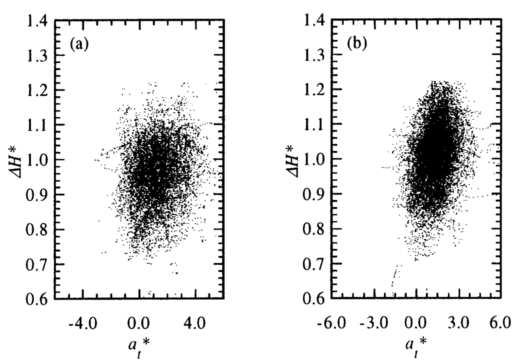

Figure 10. Scatter plots of the tangential strain rate and local heat release rate for flame elements with $Q < 0$ (a) and $Q > 0$ (b).

than that with $Q < 0$ and shows a peak at large tangential strain rate. However, pdfs of flame thickness in Fig. 9(d) are not affected by the second invariant on the flames. In Fig. 10, relation between the tangential strain rate and the local heat release rate are shown for the flame elements with $Q < 0$ and $Q > 0$. By conditioning with second invariant, the correlation between them becomes more clearly. For the flame elements with $Q > 0$, the local heat release rate increases with the increase of the tangential strain rate.

CONCLUSIONS

In this study, direct numerical simulation of H_2-air turbulent premixed flame propagating in three-dimensional homogeneous isotropic turbulence are conducted to investigate fine scale structure of turbulent premixed flames. Following conclusions are obtained from this study.

(1) The fine scale structure of turbulent premixed flames are significantly affected by the coherent fine scale eddies in turbulence. The relatively strong coherent fine scale eddies can survive behind the flame front and they are perpendicular to the flame front. In these regions, heat release rate increases. Direction of many coherent fine scales eddies near the flame front tends to be parallel to the flame front and enhance the chemical reaction. In this case, the distribution of high heat release rate show tube-like structure similar to the coherent fine scale eddies of turbulence.

(2) The probability density function of local heat release rate is nearly Gaussian with a peak at maximum heat release rate of a laminar flame, while that of the curvature of flame front is far from Gaussian and shows exponential tails for large curvature. Most of flame elements are stretched by turbulent motion in the tangential directions.

(3) Strong correlation exists between local heat release rate and curvature of flame surface. The flame elements convex toward the burnt side with large curvature tend to have high heat release rate. The correlation between local heat release rate and tangential strain rate also exist, while this is not so strong.

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