ANISOTROPIC TURBULENCE GENERATION IN TURBULENT PREMIXED FLAMES

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ABSTRACT

Direct numerical simulation of a turbulent premixed flames with a single-step irreversible Arrhenius-type reaction is performed at $u'/u_L = 0.88$, $l_t/\delta = 15.9$ and $\rho_u/\rho_b = 7.53$. Fully developed stationary wrinkled flames are obtained in a domain of 8 mm x 4 mm x 4 mm.

Turbulent fluctuations generally increase in the flame region, but streamwise component increases more than transversal components. This results in the generation of anisotropic turbulence in the flame region. Analysis based on the Favre-averaged transport equation of turbulent kinetic energy shows that pressure gradient term and pressure work term increase turbulent kinetic energy in the flame region, while diffusion and dissipation term and velocity gradient term decrease it in the flame region.

After combustion, the turbulent fluctuations of transversal components decay rapidly due to the dilatation and the increase of kinematic viscosity. However, streamwise component does not decay so much and has a value larger than before combustion. Because the stream lines are divergent where the flame is convex to the burned gas, a shear flow similar to a wake is produced in the burned gas side. It is easily supposed that a shear flow similar to a jet appears when the flame is convex to the unburned gas. These local shear flows can generate anisotropic turbulence.

INTRODUCTION

DNS plays an important role in evaluation and development of turbulent combustion models. But there are a few databases of three-dimensional turbulent premixed flames. For example, Trouvé and Poinsot (1994) calculated a propagating premixed flame in a decaying turbulence with one-step irreversible reaction, and studied the effect of Lewis numbers on statistical properties such as the turbulent burning velocity and the local flame structure. The initial characteristics of turbulence are $u'/u_L = 10.0$ and $l_t/\delta = 5.2$ and the density ratio of the flame is 4.0. Rutland and Cant (1994) also calculated a stationary premixed flame in an incoming turbulence using one-step irreversible reaction and low Mach number approximation. The initial characteristics of turbulence are $u'/u_L = 1$ and $l_t/\delta = 30$ and the density ratio of the flame is 3.3. Besides these simple reaction cases, Tanahashi et al. (1999) performed three-dimensional DNS of H_2-air turbulent premixed flames with detailed kinetic mechanism including 12 reactive species and 27 elementary reactions. The initial characteristics of turbulence are $u'/u_L = 3.0$ and $l_t/\delta = 1.74$.

Hasegawa et al. (1999) and Nishiki et al. (2000) studied turbulence, flame structure and transport properties of turbulent premixed flames on the basis of DNS with one-step irreversible reaction, though flames were not enough developed. The initial characteristics of turbulence are $u'/u_L = 4.8$ and $l_t/\delta = 8.0$ and the density ratio of the flame is 7.53. In this study, a fully developed stationary wrinkled flame is obtained in a turbulent flow of $u'/u_L = 0.88$ and $l_t/\delta = 15.9$ with a flame of $\rho_u/\rho_b = 7.53$, and anisotropic generation of turbulence is analyzed.

DIRECT NUMERICAL SIMULATION

Basic Equations

Following assumptions are used in this simulation: 1) The chemical reaction is a single-step irreversible one with heat release, where the molecular weights of reactants and products are the same. 2) The bulk viscosity, the Soret and the Dufour effects, and the pressure gradient diffusion are neglected. 3) The specific heat at constant pressure and the specific heat ratio are constant. 4) The equation of state of the burned and unburned gases is that of an ideal gas. Following the above assumptions, basic equations are written as equations (1) – (4).

Mass conservation

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_j)}{\partial x_j}=0 \qquad (1)$$

Momentum conservation

$$\frac{\partial(\rho u_i)}{\partial t}+\frac{\partial(\rho u_i u_j)}{\partial x_j}+\frac{\partial p}{\partial x_i}=\frac{\partial \tau_{ij}}{\partial x_j} \quad (i=1,2,3) \qquad (2)$$

Energy conservation

$$\frac{\partial e_t}{\partial t}+\frac{\partial\{(e_t+p)u_j\}}{\partial x_j}=\frac{\partial(u_j\tau_{kj})}{\partial x_k}-\frac{\partial q_j}{\partial x_j} \qquad (3)$$

Species conservation

$$\frac{\partial(\rho Y)}{\partial t}+\frac{\partial(\rho Y u_j)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial Y}{\partial x_j}\right)+W \qquad (4)$$

In equations (1) – (4), τ_{ij}, e_t, q_i, W are written as follows:

Stress tensor

$$\tau_{ij}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right) \qquad (5)$$

Total energy

$$e_t=\rho\, QY+\frac{\rho RT}{\gamma-1}+\frac{\rho}{2}(u^2+v^2+w^2) \qquad (6)$$

Heat flux

$$q_i=-\lambda\frac{\partial T}{\partial x_i}-\rho DQ\frac{\partial Y}{\partial x_i} \qquad (7)$$

Reaction term

$$W=-B\rho YT^{\beta}\exp\left(-\frac{\theta}{T}\right) \qquad (8)$$

where μ, λ, D are the viscosity, the thermal conductivity and the diffusion coefficient, Q is the released heat, B is the frequency factor, β is the index of temperature dependency and θ is the characteristic temperature of the activation energy. Viscosity coefficient is evaluated by the 0.7 power of temperature, while the Lewis number is 1.0 and the Prandtl number is 0.75.

Properties of Premixed Gas

A premixed gas is supposed to have the pressure of 0.1 MPa, the initial temperature of 300 K, the density of 0.942 kg/m^3, the released heat Q of 2.45 x 10^6 J/kg, the specific heat at constant pressure C_p of 1.25 x 10^3 J/kg·K, the specific heat ratio γ of 1.4, and the viscosity coefficient μ_0 of 1.77 x 10^{-5} Pa·s at the initial temperature. Thus the adiabatic flame temperature T_a is 2260 K and the density ratio of the flame ρ_u/ρ_b is 7.53. The index of temperature dependency β is 1.0, the characteristic temperature of activation energy θ is 19600 K and the laminar burning velocity u_L is set 0.600 m/s. As a result, the frequency factor B is 2.79 x 10^6 1/s·K and the flame thickness δ is 0.217 mm.

Calculation Method

Figure 1 shows the simulation domain, which is a box of 8 mm x 4 mm x 4 mm. The number of grid points is 512 in the x direction and 128 in y, z directions. The x coordinate is taken in the streamwise direction and y, z coordinates are taken in the transversal directions.

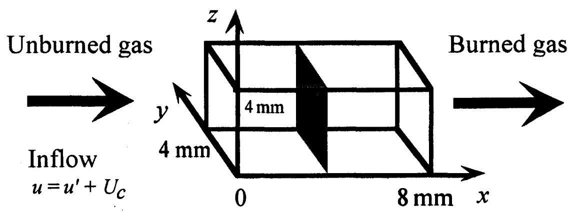


Figure 1 : Simulation domain and coordinate system.

Boundary conditions in y, z directions are periodic, and those in x direction are non-periodic to be able to treat incoming flesh turbulent mixture and outgoing burned gas. Inadequate boundary conditions for incoming and outgoing flows may produce reflecting pressure waves and false vorticity. Thus the NSCBC (Navier-Stokes Characteristic Boundary Conditions) proposed by Poinsot and Lele (1992) and Baum et al. (1994) is applied to the boundaries of the x direction. At the inflowing boundary, the velocity is assigned by assuming Taylor's hypothesis and shifting the phase of a homogeneous isotropic turbulence calculated beforehand, while non-reflecting and free boundary condition are assigned at the outgoing boundary.

The 6th-order central finite difference method is used for the x direction to treat non-periodic boundary conditions and the Fourier spectral collocation method is used for y, z direction. The 3rd-order Runge-Kutta method is used for time integration.

u'/u_L	l_t/δ	l_m/δ	l_d/δ	Re_t
0.88	15.9	9.44	0.65	95.5

u': Turbulent intensity, u_L: Laminar burning velocity = 0.60 m/s,
l_t : Integral length scale, l_m : Taylor micro scale,
l_d : Kolmogorov scale, δ : Flame thickness = 0.217 mm,
Re_t : Reynolds number based on the integral length scale.

Table 1 : Characteristics of homogeneous isotropic turbulence.

A vector-parallel computer (Fujitsu VPP 700) with 32 PEs is used for this direct numerical simulation. CPU time is about 50 hours for 1ms of real-time simulation.

Initial Conditions

Pre-calculated homogeneous isotropic turbulence listed in Table 1 is assigned for velocity field in the domain with a mean inflowing velocity of 0.60 m/s. A homogeneous isotropic turbulence is calculated by giving the following energy spectrum to satisfy incompressibility.

$$E(k) = 16u'^2_0\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\frac{k^4}{k_0^5}\exp\left\{-2\left(\frac{k}{k_0}\right)^2\right\} \qquad (9)$$

where k_0 is 6 and u'_0 is 3.87 m/s. The characteristics of the obtained homogeneous isotropic turbulence after about 2 times the turnover time are listed in Table 1. This same homogeneous isotropic turbulence comes into the domain with a mean velocity of 0.60 m/s at the inflowing boundary.

Distributions of temperature, pressure, mass fraction and expansion velocity are also given as if a planar flame is located in the simulation domain as shown in Figure 1. The mean inflowing velocity is changed on the way of the calculation to keep a developed wrinkled flame in the simulation domain.

RESULTS AND DISCUSSIONS

Wrinkled Flame

The mean inflowing velocity U_c was changed from 0.60 m/s to 1.0 m/s at t = 4.65 ms and from 1.0 m/s to 1.2 m/s at t = 9.30 ms on the way of the calculation. And then this simulation is continued till t = 15.5 ms. The contour surface of temperature drawn at 1470 K at t = 13.44 ms is shown in Figure 2. It is found that a stationary wrinkled flame appears in the turbulent flow. The flame region exists between x/L = 0.25 and 1.07, which is about 15 times larger than the laminar flame thickness. The contour surface of total vorticity drawn at 0.29 x 10^4 1/s is also shown in Figure 2. Fine scale structure of turbulence exists in the incoming turbulent flow and vorticity production occurs near the wrinkled flame, though the mechanism has not been cleared yet.

Time averaged turbulent burning velocity is 1.146 m/s after t = 9.30 ms, which is very close to u_L+u' = 1.128 m/s. The turbulent burning velocity is defined by equation (10).

$$u_T = -\frac{1}{\rho_u Y_u A_L}\int_V W dV \qquad (10)$$

where ρ_u is the density of the unburned gas, Y_u is the fuel mass fraction in the unburned gas (Y_u = 1), A_L is the area of the planar flame and W is the reaction rate.

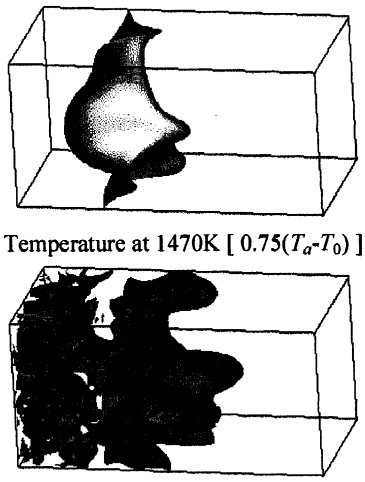


Figure 2 : Contour surfaces at t = 13.44 ms.

Generation of Anisotropic Turbulence

Figure 3 shows streamwise evolution of turbulent fluctuations at t = 13.44 ms.

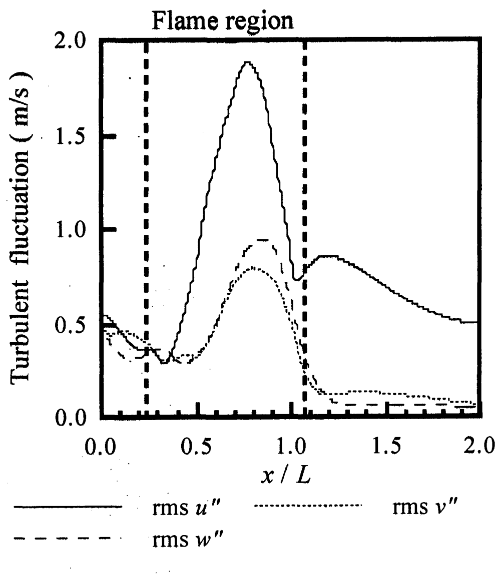
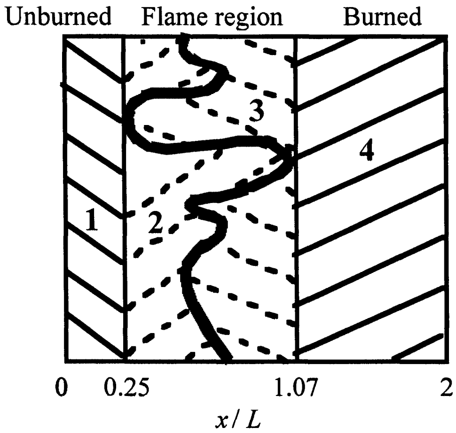


Figure 3 : Streamwise evolution of turbulent fluctuation.

The fluctuations somewhat decay in front of the flame region, but all components of turbulent fluctuations increase dramatically in the flame region, especially x component increases more than twice as much as y, z component. This results in the generation of anisotropic turbulence in the flame region.

In Figure 3, the turbulent fluctuations in the flame region may be over-estimated, because turbulent fluctuations are not calculated conditionally in the unburned gas and in the burned gas. In order to estimate correctly the generation of turbulent fluctuations, turbulent fluctuations are calculated conditionally in the 4 parts as shown in Figure 4.



Part 1: Unburned gas area
Part 2: Unburned gas area in the flame region
Part 3: Burned gas area in the flame region
Part 4: Burned gas area

Figure 4 : Separated domain.

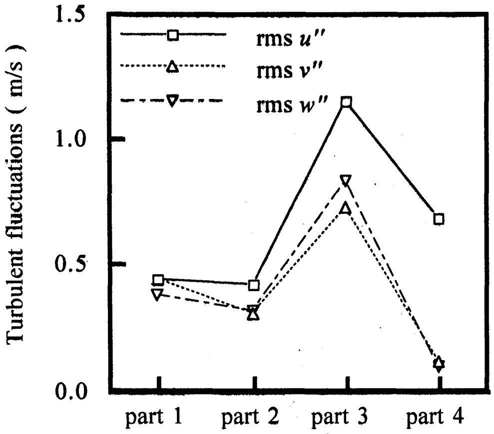


Figure 5 : Evolution of turbulent fluctuations calculated conditionally.

Figure 5 shows evolution of turbulent fluctuations, which are calculated conditionally. It is shown that turbulent fluctuations of all components are amplified in the turbulent flame region, and an anisotropic turbulence is generated because x component are produced more than y, z components. After combustion, y, z components of turbulent fluctuation decay rapidly due to the dilatation and the increase of kinematic viscosity. However, x component does not decay so much and has a value larger than before combustion.

Generation of Turbulent Kinetic Energy in the Flame Region

The mechanism of turbulence generation in the flame region is analyzed on the basis of the Favre-averaged transport equation of turbulent kinetic energy along streamwise direction. The transport equation is written as follows:

$$\frac{\partial \tilde{k}}{\partial t} + \tilde{u}_k \frac{\partial \tilde{k}}{\partial x_k} = \underbrace{-\frac{\overline{\rho u_i'' u_k''}}{\bar{\rho}} \frac{\partial \tilde{u}_i}{\partial x_k}}_{(\mathrm{I})} \underbrace{-\frac{1}{\bar{\rho}} \frac{\partial \overline{\rho u_i'' u_i'' u_k''}}{2 \partial x_k}}_{(\mathrm{II})}$$

$$\underbrace{-\frac{\overline{u_i''}}{\bar{\rho}} \frac{\partial \bar{p}}{\partial x_i}}_{(\mathrm{III})} \underbrace{-\frac{1}{\bar{\rho}} \overline{u_i'' \frac{\partial p'}{\partial x_i}}}_{(\mathrm{IV})} \underbrace{+\frac{1}{\bar{\rho}} \overline{u_i'' \frac{\partial \tau_{ik}}{\partial x_k}}}_{(\mathrm{V})} \qquad (11)$$

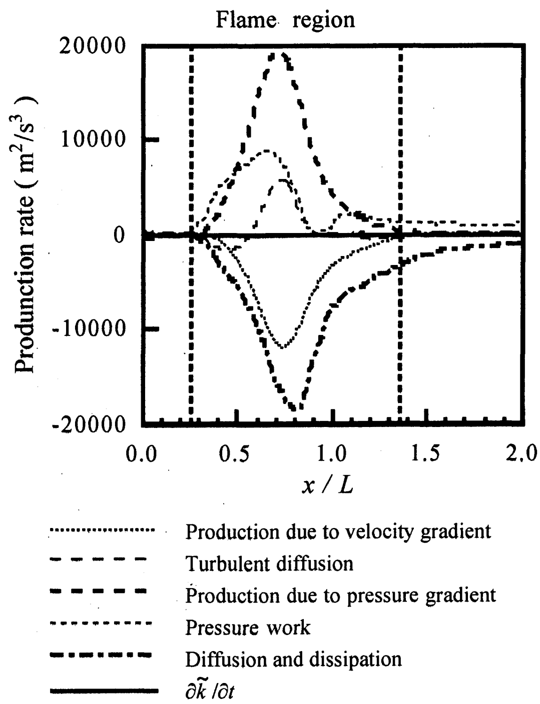


Figure 6 : Streamwise balance of the production rate of turbulent kinetic energy. Flame region is defined between 0.01 and 0.99 of averaged progress variable. $\partial \tilde{k}/\partial t$ is calculated from the transport equation by subtracting the convection term from the right hand side.

where term (I) is the production due to velocity gradient, term (II) is the turbulent diffusion, term (III) is the production due to pressure gradient, term (IV) is the pressure work and term (V) is the diffusion and the dissipation. Evolution of each term, which is averaged between t = 9.30 ms and t = 15.50 ms, is shown in Figure 6. It is found that the pressure gradient term and the pressure work term produce kinetic energy in the flame region, while the diffusion and dissipation term and the velocity gradient term decrease it.

Mechanism of Anisotropic Turbulence Generation behind Flame

In order to understand the mechanism of anisotropic turbulence generation behind the flame, the stream lines crossing the section of y / L = 0.5 are visualized as shown in Figure 7. The stream lines are divergent where the flame is convex to the burned gas. As a result, a shear flow similar to a wake is produced behind flame. The distribution of velocity of u, v, w at x / L = 1.5 (A-B in Figure 7) is shown in Figure 8. Streamwise velocity u has a difference about 2.4 m/s between minimum value to maximun value, while transversal velocities v, w have discrepancies of only 0.1 m/s. This results in the generation of anisotropic turbulencec after combustion, which is shown in Figure 3. It is easily supposed that a shear flow similar to a jet appears when the flame is convex to the unburned gas. These local shear flows can generate anisotropic turbulence.

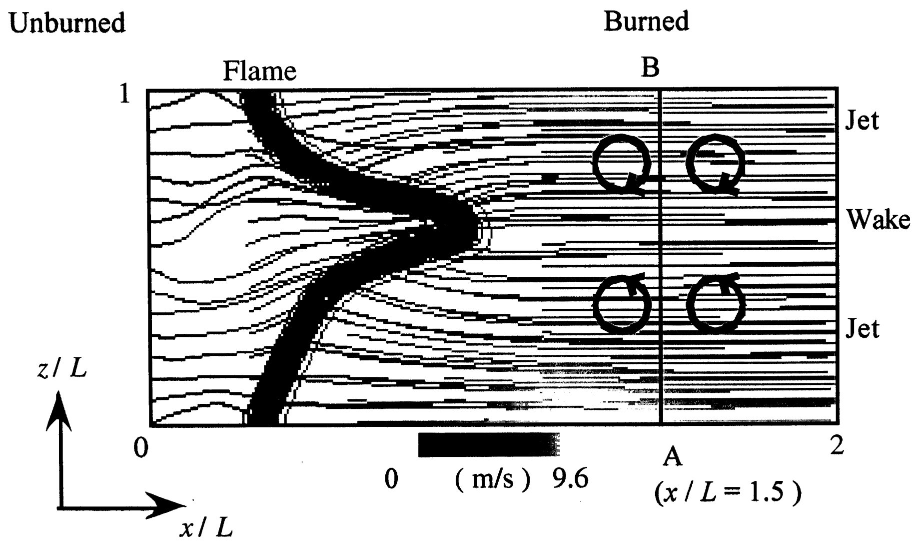


Figure 7 : Stream lines curved by the flame at the section of y / L = 0.5.

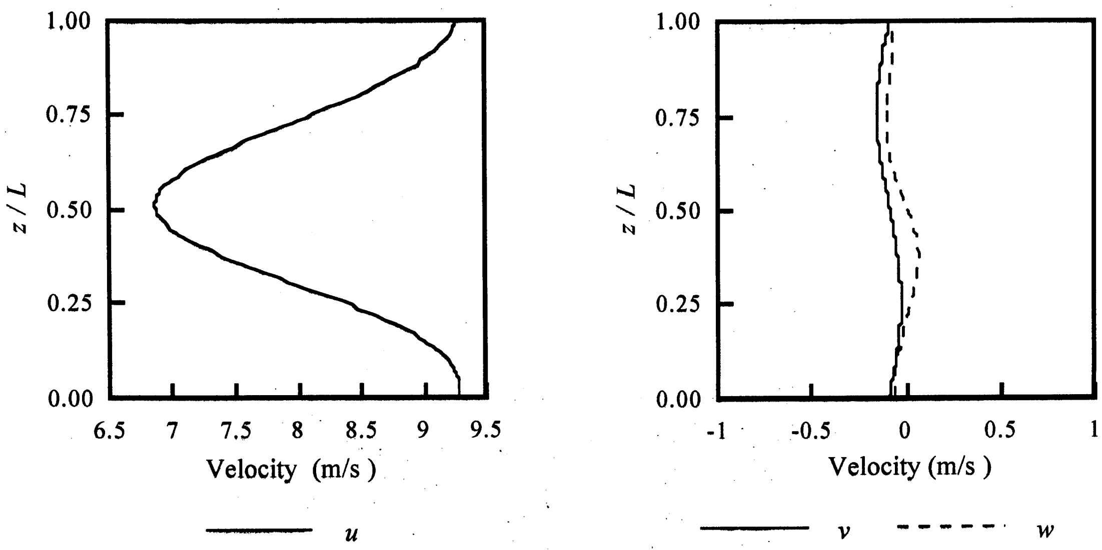


Figure 8 : Distribution of velocity on x / L =1.5 (A-B in Figure 7) at the section of y / L = 0.5.

CONCLUSIONS

A fully developed stationary wrinkled flame in a homogeneous turbulence flow is directly simulated with a single-step irreversible reaction. Following conclusions are obtained.

(1). Turbulent fluctuations of all components are amplified in the flame region, and an anisotropic turbulence is generated because streamwise component are produced more than transversal ones.

(2). Behined the flame, turbulent fluctuations of transversal components decay rapidly due to the dilatation and the increase of kinematic viscosity. However, x component does not decay so much and has a value larger than before combustion.

(3). Analysis based on the Favre-averaged transport equation of turbulent kinetic energy shows that pressure gradient term and pressure work term increase turbulent kinetic energy in the flame region, while diffusion and dissipation term and velocity gradient term decrease it.

(4). Stream lines are curved by the wrinkled flame and local shear flows like a wake or a jet appear behind wrinkled flames. These local shear flows can generate anisotropic turbulence.

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