DNS and Modeling for Turbulent Premixed Combustion

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Turbulent Premixed Combustion is very complicated physics phenomenon, mixed turbulence and combustion. That's why building turbulent premixed combustion models for numerical prediction is quite difficult. Flame Generated Turbulence which was first proposed by Karlovitz, et al. [1], and Counter-gradient diffusion which was discussed by Libby and Bray [2] are particular phenomena in turbulent premixed combustion, and they must be included in turbulent premixed combustion modelling. In order to progress toward understanding the importance of this phenomenon, structures and characteristics of turbulent premixed flames are progressively made clear experimentally and modelled [3, 4 et al.]. However, it is impossible to measure all variables in time and in space experimentally. Therefore DNS takes an important place in order to evaluate and develop turbulent combustion models. After the 1990's, the direct numerical simulation (DNS) has been proved to have important roles on the quantitative evaluation of physics and models of turbulent premixed flames (early DNS; Trouvé and Poinsot [5], Rutland and Cant [6], Zhang and Rutland [7], Tanahashi et al. [8-10]). However, turbulent combustion model is not fully developed now.

In our past study, we constructed DNS databases of fully developed turbulent premixed flames under different flame conditions as shown in Table 1 (ρ_u/ρ_b = 7.53, 5.00, 2.50), while relatively weak turbulence intensity nearly equal to the laminar burning velocity. The simulation domain is a box of 8mm x 4mm x 4mm as shown in figure 1. The x coordinate represents the streamwise direction and an unburned gas of precalculated turbulence velocity field comes into the domain from left side boundary, and burned gas goes out through the right side boundary. For the spatial derivative, the sixth-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 the y, z directions of periodic boundary conditions. Boundary conditions in the x direction are non-periodic, and then the NSCBC (Navier-Stokes Characteristic Boundary Conditions) [11, 12] are applied. For the time integration, a third-order three-step Runge-Kutta method is used. The following assumptions are made for DNS of turbulent premixed combustion with compressibility, viscosity and heat release. (1) the chemical reaction is a single-step irreversible one with heat release, (2) The bulk viscosity, the Soret and the Dufour effects, and the pressure gradient diffusion can be neglected, (3) The specific heat at constant pressure and the specific heat ratio are constant, (4) The equation of state for the burned and unburned gases is ideal, (5) The transport coefficients are temperature dependent, as follows: $\mu = \mu_0(T/T_0)^{0.7}$, $Le = (\lambda/\rho D C_p) = 1.0$, $Pr = (\mu C_p/\lambda) = 0.75$. These flame characteristics are shown in Table 1. Snapshots of temperature are shown figure 2. Then we constructed databases of fully developed turbulent premixed flames, and flame-generated turbulence and counter gradient diffusion are observed.

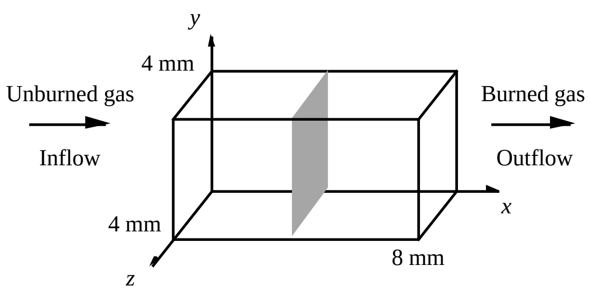


Fig. 1. Simulation domain and coordinate systems.

Table 1. Properties of flames.

	Case H	Case M	Case L
ρ_u/ρ_b	7.53	5.00	2.50
T_a	2260 K	1500 K	750 K
u_L	0.600 m/s	0.523 m/s	0.416 m/s
e_L	0.217 mm	0.191 mm	0.158 mm

T_a: adiabatic temperature, u_L: laminar burning velocity, e_L: laminar flame thickness.

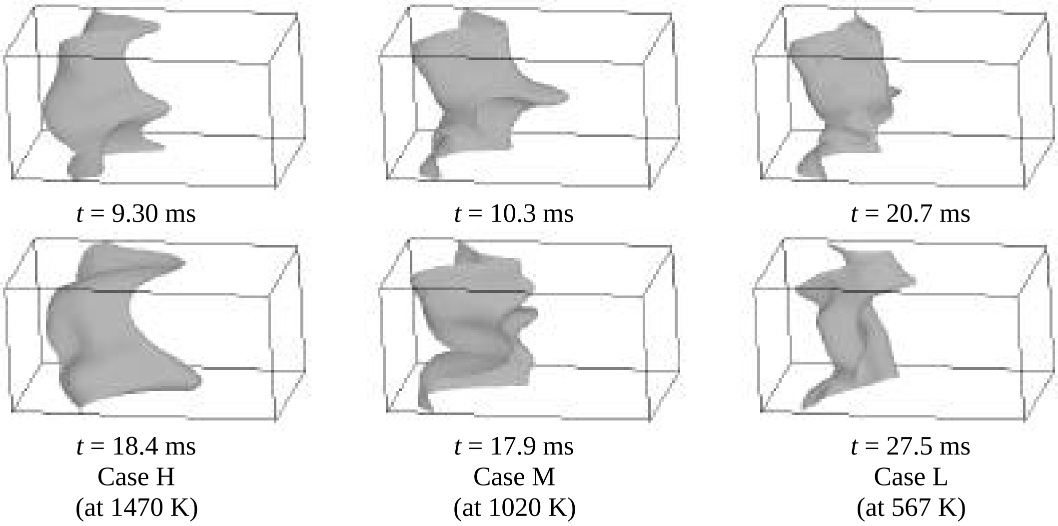


Fig. 2 Temporal evolution of wrinkled flames, contour surfaces at about c = 0.6.

The Favre-averaged transport equation for turbulent kinetic energy is written as follows:

$$\frac{\partial \tilde{k}}{\partial t} + \tilde{u}_k \frac{\partial \tilde{k}}{\partial x_k} = \underbrace{-\frac{\overline{\rho u_i'' u_k''}}{\bar{\rho}}\frac{\partial \tilde{u}_i}{\partial x_k}}_{\text{(I)}} \underbrace{-\frac{1}{\bar{\rho}}\frac{\partial \overline{\rho u_i'' u_i'' u_k''}}{2\partial x_k}}_{\text{(II)}} \underbrace{-\frac{\overline{u_i''}}{\bar{\rho}}\frac{\partial \bar{p}}{\partial x_i}}_{\text{(III)}} \underbrace{-\frac{1}{\bar{\rho}}\overline{u_i''\frac{\partial p'}{\partial x_i}}}_{\text{(IV)}} + \underbrace{\frac{1}{\bar{\rho}}\overline{u_i''\frac{\partial \tau_{ik}}{\partial x_k}}}_{\text{(V)}} \tag{1}$$

where (I) is the mean velocity gradient, (II) is turbulent diffusion, (III) is mean pressure gradient, (IV) is pressure work, (V) is diffusion and dissipation term. Analysis based on this equation showed that pressure-related terms produced kinetic energy in the flame brush for all cases. Streamwise evolutions for each term are shown in Fig. 3.

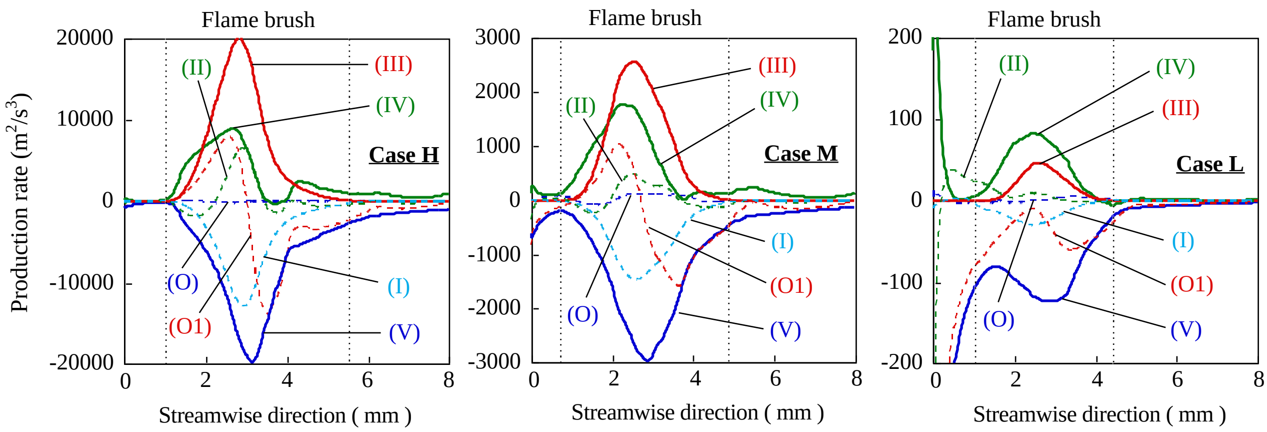


Fig. 3 Streamwise balance of the production rate of turbulent kinetic energy

The Favre-averaged transport equation for the turbulent scalar flux is written as follows:

$$\frac{\partial \overline{\rho u_j'' c''}}{\partial t} + \frac{\partial}{\partial x_i}\left(\overline{\rho u_j'' c''}\tilde{u}_i\right) = \underbrace{-\frac{\partial}{\partial x_i}\left(\overline{\rho u_i'' u_j'' c''}\right)}_{\text{(A)}} \underbrace{-\overline{\rho u_j'' u_i''}\frac{\partial \tilde{c}}{\partial x_i}}_{\text{(B)}} \underbrace{-\overline{\rho c'' u_i''}\frac{\partial \tilde{u}_j}{\partial x_i}}_{\text{(C)}}$$

$$\underbrace{-\overline{c''}\frac{\partial \bar{p}}{\partial x_j}}_{\text{(D)}} \underbrace{-\overline{c''\frac{\partial p'}{\partial x_j}}}_{\text{(E)}} + \underbrace{\overline{u_j''\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial c}{\partial x_i}\right)} + \overline{c''\frac{\partial \tau_{ji}}{\partial x_i}}}_{\text{(F)} \quad \text{(G)}} + \underbrace{\overline{\rho u_j'' \dot{\omega}}}_{\text{(H)}} \tag{2}$$

where, (A) is the transport term by turbulence, (B) is the mean progress variable gradient term, (C) is the mean velocity gradient term, (D) is the mean pressure gradient term, (E) is the fluctuating pressure term, (F) is the dissipation term due to diffusivity, (G) is the dissipation term due to viscosity, and (H) is the velocity-reaction rate correlation term. Analysis based on this equation showed that the mean pressure gradient term, the velocity-reaction rate correlation term and the fluctuating pressure term played important roles in the production of countergradient diffusion, while the mean velocity gradient term, the mean progress variable gradient term and the dissipation terms suppressed the production of countergradient diffusion. Streamwise evolutions for each term are shown in Fig. 4.

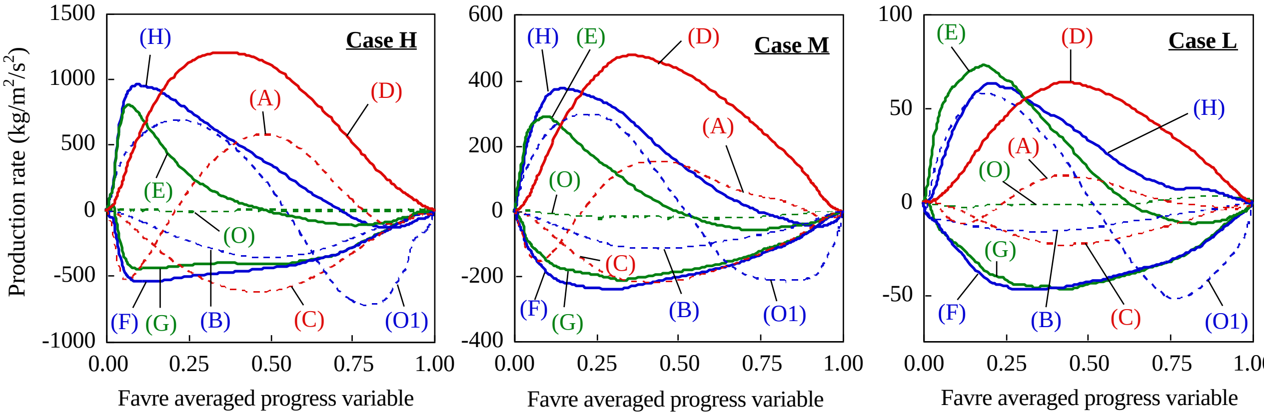


Fig. 4 Streamwise balance of the production rate of turbulent scalar flux as a function of mean progress variable

Pressure work term (IV) and diffusion and dissipation term (V) can be decomposed as follows;

$$\underbrace{-\frac{1}{\bar{\rho}}\overline{u_i''\frac{\partial p'}{\partial x_i}}}_{\text{(IV)}} = \underbrace{-\frac{1}{\bar{\rho}}\frac{\partial \overline{p'u_i''}}{\partial x_i}}_{\text{(IV1)}} + \underbrace{\frac{1}{\bar{\rho}}\overline{p'\frac{\partial u_i''}{\partial x_i}}}_{\text{(IV2)}} \tag{3}$$

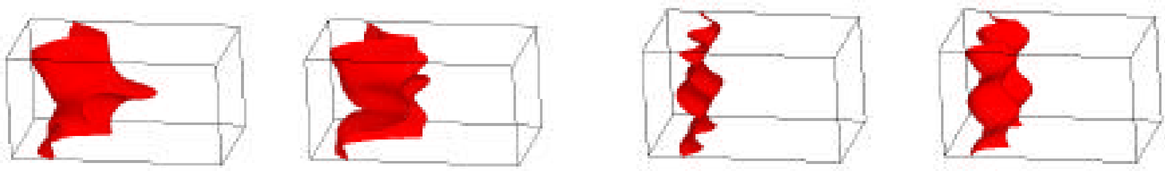
$$\underbrace{\frac{1}{\bar{\rho}}\overline{u_i''\frac{\partial \tau_{ik}}{\partial x_k}}}_{\text{(V)}} = \underbrace{-\frac{1}{\bar{\rho}}\mu\overline{\frac{\partial u_i''}{\partial x_k}\frac{\partial u_i''}{\partial x_k}}}_{\text{(V1)}} + \underbrace{\frac{1}{\bar{\rho}}\overline{u_i''\frac{\partial\left(\mu\partial u_k''/\partial x_i\right)}{\partial x_k}}}_{\text{(V2)}} \underbrace{-\frac{2}{3}\frac{1}{\bar{\rho}}\overline{\frac{\partial\left(\mu\partial u_\gamma''/\partial x_\gamma\right)}{\partial x_k}u_k''}}_{\text{(V3)}} + \Delta \tag{4}$$

where (IV1) pressure diffusion term and (IV2) pressure dilatation term, and (V1) classical dissipation term (V1), (V2), (V3) additional dissipation components, and other small terms.
We modelled combustion related terms, (III), (IV2) and (V2)+(V3) terms in transport equation for turbulent kinetic energy, and (D), (E), (F), (G) and (H) terms in transport equation for the turbulent scalar flux

Above DNS results are in condition of relatively weak turbulence intensity nearly equal to the laminar burning velocity. We are trying to construct new DNS databases in higher turbulence intensity. Now we have not yet gotten it, but one of the result of DNS are shown as follows.

New DNS of turbulent premixed flames while the turbulence conditions of twice of turbulent intensity and the half of integral length scale compared with previous cases is executed under the density ratio of ρ_u/ρ_b = 5.00 and DNS databases of statistically fully developed steady turbulent flames are obtained. Based on new DNS databases, the transport equation for turbulent kinetic energy are analyzed and distributions of each term show similar evolution between previous and new DNS results.

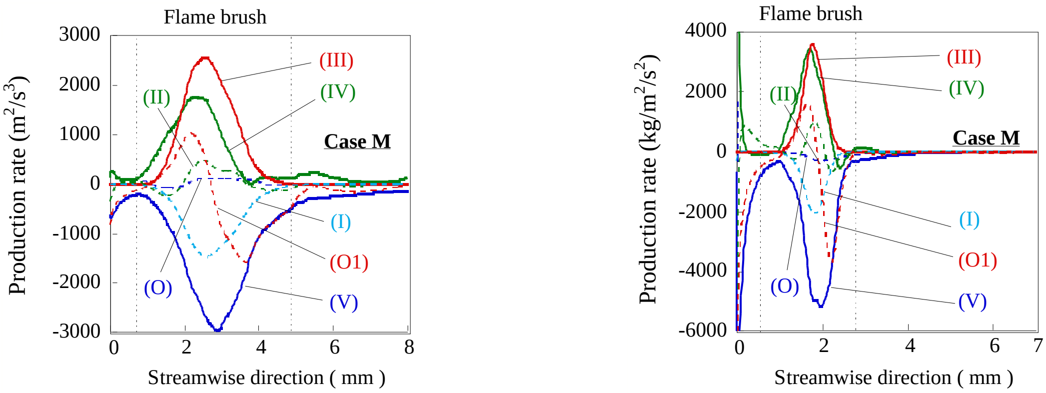
Snapshots of temperature are shown in Fig. 5. New DNS results show the depth of wrinkled flame becomes smaller then previous one. And streamwise evolutions in transport equation for turbulent kinetic energy Eq. (1) for each term are shown in Fig. 6. Both of previous and new DNS results show the pressure gradient term (III) and pressure work term (IV) produce kinetic energy in the flame region, while diffusion and dissipation term (V) and velocity gradient term (I) decrease it.



t = 10.3 ms t = 17.9 ms t = 13.4 ms t = 21.3 ms

(a) Case M with u' = 0.526 m/s (previous results) (b) Case M with u' = 1.05 m/s (new results)

Fig. 5 Contour surfaces of temperature 1020 K.



(a) Case M with u' = 0.526 m/s (previous results) (b) Case M with u' = 1.05 m/s (new results)

Fig. 6 Streamwise balance of the production rate of the turbulent kinetic energy.

We continue to execute DNS in higher and realistic turbulence conditions to construct DNS databases for the modelling of turbulent combustion. This is not future work, but underway work at present.

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1: Nishiki S., Hasegawa T., Borghi R., Himeno R., Modeling of Flame-Generated Turbulence Based on Direct Numerical Simulation Databases, Proc. Comb. Inst. **29**, 2017-2022, 2002.

2: Nishiki S., Hasegawa T, Borghi R., Himeno R., Modelling of turbulent scalar flux in turbulent premixed flames based on DNS databases, Combustion Theory and Modelling, **10**-1, 39-55, 2006.