Direct Numerical Simulation of Chemically Reacting Mixing Layers*

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The objective of this paper is to gain insight into the process of chemical reaction in turbulent mixing layers. To achieve this purpose, we have performed direct numerical simulations of three-dimensional chemically reacting mixing layers using a spectral method. The results are reported for the case of velocity fields with initial periodic excitation. From these results, we have reached the following conclusions: 1) on the streamwise vortical structures (ribs) in the braid region, the peak of the chemical production term exists; and 2) the core region contributes significantly to the total production in the mixing layer, whereas local production rate is not so high.

Key Words: Computational Fluid Dynamics, Numerical Analysis, Direct Numerical Simulation, Turbulence, Mixing, Coherent Structure, Spectral Method, Reactive Flow

1. Introduction

It is very important to clarify the mechanism of chemical reaction in turbulent shear layers. From the industrial viewpoint, these reacting flows are fundamental to understanding turbulent diffusion flames. Since the discovery of the two-dimensional coherent vortical structure and three-dimensional rib structure in turbulent mixing layers^{(1),(2)}, many studies have been conducted to clarify the effect of these coherent structures on chemical reactions^{(3),(4)}. As the entrainment and mixing processes in the turbulent mixing layer are controlled by the coherent vortical structure, understanding the coherent structure is essential in explaining the mechanism of chemical reaction in turbulent mixing layers. The authors have conducted large eddy simulations (LES) of a turbulent mixing layer, and expounded the coherent vortical structure and turbulent mixing process^{(5),(6)}. To apply LES to the

chemically reacting flow field, however, improvement of the subgrid scale model is necessary.

In this paper, the direct numerical simulations of chemically reacting mixing layers using a spectral method were conducted for the cases with initial periodic excitation. The objective of this study is to gain insight into the relationship between the chemical reaction and the coherent structure.

2. Nomenclature

- c_i : Mass fraction of species i
- c_{i0} : Mass fraction of species i in the main stream
- E_i : Power spectrum of variable i
- k_i : Wave number in the i direction
- L_0 : Reference length scale
- N_i : Fourier mode in the i direction
- P : Nondimensional total pressure
 $= p + (1/2)u^2$
- R : Reaction rate coefficient
- Re : Reynolds number
- Sc : Schmidt number
- u : Nondimensional velocity vector
- u : Nondimensional velocity component in x direction

* Received 14th May 1992. Paper No. 91-0217 A

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- u_i : Nondimensional velocity component in the i direction
 Δt : Nondimensional time step
 v : Nondimensional velocity component in y direction
 w : Nondimensional velocity component in z direction
 x : Nondimensional space coordinate
 y : Nondimensional space coordinate
 z : Nondimensional space coordinate
 α : Most unstable wave number for hyperbolic tangent velocity profile
 ζ : Coordinate in z direction nondimensionalized by the grid space
 η : Coordinate in y direction nondimensionalized by the grid space
 ξ : Coordinate in x direction nondimensionalized by the grid space
 τ : Nondimensional time
 ω : Nondimensional vorticity vector
 ω_i : Nondimensional vorticity component in i direction

3. Fundamental Equations and Numerical Method

In this study, reactions such as $A + B \rightarrow P$ are considered. We assume that heat release with chemical reaction is negligible, so that chemical species can be treated as a passive scalar. The fundamental equations follow the unsteady three-dimensional incompressible Navier-Stokes equations, mass conservation equation and chemical species conservation equations are:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \times \mathbf{u} = -\nabla P + \frac{1}{Re} \nabla^2 \mathbf{u} \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

$$\frac{\partial C_A}{\partial t} + \mathbf{u} \cdot \nabla C_A = \frac{1}{ReSc} \nabla^2 C_A - RC_{ACB} \quad (3)$$

$$\frac{\partial C_B}{\partial t} + \mathbf{u} \cdot \nabla C_B = \frac{1}{ReSc} \nabla^2 C_B - RC_{ACB} \quad (4)$$

$$\frac{\partial C_P}{\partial t} + \mathbf{u} \cdot \nabla C_P = \frac{1}{ReSc} \nabla^2 C_P + 2RC_{ACB} \quad (5)$$

where C_A , C_B and C_P represent mass fractions.

We applied a spectral method to this problem by expanding the velocity and concentrations fields in a Fourier series as follows:

$$u_j(\mathbf{x}, t) = \sum_{k_1=-\frac{N_1-1}{2}}^{\frac{N_1-1}{2}} \sum_{k_3=-\frac{N_3-1}{2}}^{\frac{N_3-1}{2}} \sum_{k_2=0}^{N_2} \hat{u}_j(\mathbf{k}, t) \times e^{ik_1x_1} e^{ik_3x_3} \begin{cases} \cos k_2x_2 & j=1, 3 \\ \sin k_2x_2 & j=2 \end{cases} \quad (6)$$

$$c_j(\mathbf{x}, t) = \sum_{k_1=-\frac{N_1-1}{2}}^{\frac{N_1-1}{2}} \sum_{k_3=-\frac{N_3-1}{2}}^{\frac{N_3-1}{2}} \sum_{k_2=0}^{N_2} \hat{c}_j(\mathbf{k}, t) \times e^{ik_1x_1} e^{ik_3x_3} \cos k_2x_2 \quad (7)$$

where subscripts 1, 2 and 3 represent x , y and z components respectively. The spatial derivatives are computed in Fourier space, but nonlinear terms are evaluated in physical space, where aliasing errors are removed by a padding method. The initial condition for the mean streamwise velocity is defined by a hyperbolic tangent velocity profile,

$$\frac{U(y)}{U_0} = \tanh\left(\frac{2\pi}{\alpha} y\right) \quad (8)$$

where $\alpha=0.4446$ is the most unstable wave number for the hyperbolic tangent velocity profile, which is obtained from the Rayleigh equation.

On the mean velocity profile, fundamental and subharmonic modes of the solution of the Rayleigh equation and periodic spanwise disturbance were superposed⁽⁷⁾. We set fluctuation intensity at $y=0$ equal to 2.8%, 1.4% and 1.4% of the mean velocity difference for fundamental, subharmonic and three-dimensional modes, respectively. As for the wavelength of spanwise disturbance, we adopted 2/3 of the fundamental wavelength because the streamwise vorticity in the braid region develops most rapidly⁽⁷⁾. As for the initial concentration profile, the following profiles are selected:

$$\frac{C_A(y)}{C_{A0}} = 0.5 + 0.5 \tanh\left(\frac{2\pi}{\alpha} y\right) \quad (9)$$

$$\frac{C_B(y)}{C_{B0}} = 1.0 - \frac{C_A(y)}{C_{A0}}, \quad (10)$$

where $C_{A0} = C_{B0} = 1$. The initial mean velocity profile and the initial concentration profile are shown in Fig. 1.

The computational domain was chosen to be 16 cm $\times$ 16 cm $\times$ 16 cm, and the calculation was performed in 32 $\times$ 33 $\times$ 32 and 64 $\times$ 65 $\times$ 64 grid points. Consequently, N_i in Eqs. (6) and (7) becomes 32 or 64. Periodic boundary conditions were used for the streamwise (x) and spanwise (z) directions, and free-slip boundary conditions were applied for the transverse (y) direction. One-half the velocity difference of mean flow was used as the reference velocity, and the half-length of the calculation domain (wavelength of fundamental mode) was selected as the reference

Fig. 1 Initial mean velocity profile and concentration profile

length scale. Physical properties of air at 0.1 MPa, and 300 K were used. Calculations were conducted for cases with Reynolds number = 700, Schmidt number = 1, 0.6, 0.2, 0.1 and the reaction rate coefficient $R = 0, 1$.

Time advancement of the convective term and pressure term was effected by using the Adams-Bashforth method and the backward Euler method, respectively. The viscous term and diffusion term were integrated by using the Crank-Nicholson method. We introduce nondimensional parameters ξ, η, ζ and τ . ξ, η , and ζ are coordinates nondimensionalized by grid spaces, and correspond to the x, y and z directions. τ indicates time nondimensionalized by the time step increment Δt .

4. Numerical Results and Discussions

First, to estimate the effect of the Schmidt number, calculations were conducted for cases of $Sc = 1, 0.6, 0.2, 0.1$. Figure 2 shows the power spectrum of the mass fraction of species A for the case of $Sc = 1$ and $R = 0$ by using $64 \times 65 \times 64$ grid points. Figure 3 shows the power spectra of velocity components u, v , and w , and total pressure P . From Figs. 2 and 3, velocity fluctuations appear to be within the limit of the spatial resolution, while concentration fluctuations contain relatively large energy in the high wave number region. High wave number fluctuation of the concentration causes lack of spatial resolution. This means that higher resolution is required for the concentration field than the velocity field for $Sc = 1$.

Figure 4 shows the power spectrum of the mass fraction of species A with chemical reaction at $\tau = 300$ for $Sc = 0.6, 0.2, 0.1$. Low spatial resolution ($32 \times 33 \times 32$ grid points) is used for these calculations. From these figures, it can be seen that much energy is contained in the high wave number region for $Sc = 0.6$, but sufficient spatial resolution is obtained for $Sc = 0.2$ and 0.1 . The linear theory⁽⁸⁾ has indicated that the spectrum distribution of the passive scalar depends significantly on Schmidt number. Hence, it is very important to maintain high spatial resolution for the

Fig. 2 Power spectrum of c_A at $\tau = 450$

case of high Schmidt number. From the above discussions, we selected the case of $Sc = 0.2$ to expound the relationship between the chemical reaction and the

(a) u

(b) v

(c) w

(d) P

Fig. 3 Power spectra of velocity component and pressure (Grid points: $64 \times 65 \times 64$)

Fig. 4 Power spectrum of c_A with chemical reaction at $\tau=300$ Fig. 5 Contour plots of spanwise vorticity ω_z , product P and production term RC_{AB} in the $x-y$ plane

coherent structure. The spatial resolution is sufficient for concentration fluctuations at $Sc=0.2$.

To clarify the relationship between chemical reaction and coherent structure, contour plots of spanwise vorticity ω_z , product P and chemical production term R_{CACB} on the $x-y$ plane are shown in Fig. 5. With the roll-up and merging of the spanwise coherent vortex, the product concentration shows a high value in the central region of the coherent vortex (core region). However, the chemical production term shows a large value in the middle region between the coherent vortices (braid region). This means that active reaction occurs in the braid region, while the reaction in the core region is not so active. Figures 6 and 7 show contour plots of streamwise vorticity ω_x and chemical production term in the $y-z$ plane. In the braid region, counterrotating vortex pairs (ribs) are formed by the three-dimensional instability of the mixing layers. These ribs are engulfed by the coherent vortical structure⁽⁷⁾ and jut out over the core region. The rib structure incurvates the concentration distribution of the reactant and increases the reaction rate in the braid region.

Figure 8 shows the transverse distribution of the

spanwise averaged chemical production term at $\tau=300$. In this figure, the mean reaction rates in the braid region ($\xi=0$) and core region ($\xi=16$) are shown. From this figure, the contribution of the coherent vortex and rib on the mean reaction rate can be identified. Figure 5 indicates that the chemical reaction occurs more actively in the rib region than in the core region. When averaged in the z direction, the mean reaction rate in the core region is comparable with that in the braid region. This shows that the contribution of the core region to the overall reaction

Fig. 7 Contour plots of streamwise vorticity ω_x and production term at $\xi=16$

Fig. 6 Contour plots of streamwise vorticity ω_x and production term at $\xi=0$

Fig. 8 Transverse distribution of spanwise-averaged R_{CACB} for $Sc=0.2$

Fig. 9 Transverse distribution of spanwise-averaged $R_{C_{ACB}}$ for $Sc=0.1$

rate is large. This is because the ribs exist intermittently in the spanwise direction, so the contribution to the overall reaction rate is not very large.

Figure 9 shows the same profile as in Fig. 8 for the case of $Sc=0.1$. In the case of $Sc=0.1$, the reaction rate in the braid region increases because of the diffusion effect, although the mean reaction rate in the core region does not change significantly with the change of diffusivity. This is because the gradient of chemical species in the braid region is larger than that in the core region.

5. Conclusions

To clarify the relationship between the chemical reaction and turbulent coherent structure for the case of mixing and reacting two-component fluids, a three-dimensional direct numerical simulation of the mixing layer with a chemical reaction was conducted using a spectral method. From this study, the following conclusions were reached.

(1) In the rib region, chemical reaction actively occurs, and the peak of the reaction term exists in the rib region.

(2) In the core region, chemical reaction is not very active, but the contribution to the overall reac-

tion is significant in this region.

Acknowledgement

This study was partly supported by the Japan Ministry of Education, Science and Culture, Grant-in-Aid for Scientific Research (Grant No. 02650149).

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