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A NUMERICAL ANALYSIS OF THE STRUCTURE OF A TURBULENT HYDROGEN JET LIFTED FLAME

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This paper presents a direct numerical simulation (DNS) study of the flame structure of a turbulent hydrogen jet lifted flame. The diameter of the hydrogen injector is 2 mm, and the injection velocity is 680 m/s. The time-dependent three-dimensional simulation was made with full chemical kinetics and rigorous transport properties. More than 22 million grid points were used. The numerical analysis, in terms of the normalized flame index, has made clear that the lifted flame is not a single flame, but a complex flame consisting of three flame elements: (1) a stable laminar leading-edge flame, (2) a conical inner vigorous turbulent premixed flame, and (3) a number of floating diffusion flame islands, surrounding the inner premixed flame. The stable laminar leading-edge flame of ring shape is stabilized outside the turbulent jet and has a triple flamelike structure with the normalized flame index around unity, indicating that the incoming flow almost balances with the laminar burning velocity. The floating flame islands are produced by turbulent behavior and local extinction of the inner premixed flame. The detached gas volume flows downstream, continuing to burn by the molecular diffusion of oxidizers. The inner rich premixed flame is strongly turbulent by the instability of the hydrogen jet at the tip. The flame is strongly stabilized by the leading-edge flame, and the heat release layer of the flame is deviated from the hydrogen consumption layer, indicating that the turbulence modifies the inner flame structure. The respective flame elements have their own complicated three-dimensional structure, and further studies are required to understand in detail the structure and stability of the lifted flame. The present study has revealed that this kind of DNS study is very useful to investigate various very complicated flame structures, such as the lifted flame.

Introduction

The lifted flame is one of the most important and interesting flame configurations from the viewpoint of fundamental and practical research. In particular, the structure and the stabilization of lifted flames have been investigated enthusiastically, from the viewpoints of flamelet extinction [1] and triple flame structure [2–5]. Most of the former works, however, are based on two-dimensional theories and simulations, and therefore the details of the flame structure and the stabilization mechanism have not been revealed yet, especially for three-dimensional and turbulent lifted flames.

The authors have been simulating a hydrogen/air turbulent jet flame by the direct numerical simulation (DNS) approach and succeeded in capturing the lifted flame solution [6]. The time-dependent three-dimensional simulations have been made with full chemical kinetics and rigorous transport properties. The computation, with more than 22 million grid points, has been conducted using the vector parallel computer numerical wind tunnel at the National Aerospace Laboratory of Japan.

From observations of simulated complicated combustion flowfields and short-term ($\simeq$0.1 ms) unsteady flame behavior, important and interesting aspects of the lifted flame have been revealed. In this paper, the structure of the lifted flame is investigated first, and three flame elements are introduced. Then various phenomena related to the respective flame elements is discussed.

Flame Configurations

The flame configuration followed the experiment by Cheng et al. [7]. A hydrogen jet is injected into

still air from a round nozzle whose diameter D is 2 mm. The jet velocity is 680 m/s, the Mach number is 0.54, and the Reynolds number based on the diameter is 13,600. In the experiment, a lifted flame with a liftoff height of 7D was observed.

Computational Model

The nine-species (H_2, O_2, OH, H_2O, H, O, H_2O_2, HO_2, and N_2) and 17-reaction model by Westbrook [8] is employed. The air is assumed to be composed of 22% O_2 and 78% N_2 in volume. The diffusion flux is evaluated using Fick's law with binary diffusion coefficients. The transport coefficients of each chemical species, namely, viscosity μ_s, heat conductivity κ_s, and binary diffusion coefficient D_s, are evaluated using the Lennard-Jones intermolecular potential model [9], and those of the gas mixture are calculated by Wilke's empirical rule [10]. The enthalpy of each chemical species is derived from JANAF [11].

Governing Equations

The governing equations are the compressible three-dimensional Navier-Stokes equations, the conservation equations of total energy and chemical species, and the equation of state. The equation of total mass conservation is solved additionally. They are written for a generalized curvilinear coordinate system as

$$\frac{\partial Q}{\partial \tau} + \frac{\partial F_{\xi_i}}{\partial \xi_i} = \frac{\partial F_{v\xi_i}}{\partial \xi_i} + H_c, \tag{1}$$

with

$$Q = V\begin{bmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho u_3 \\ E \\ \rho z_s \end{bmatrix} \qquad F_{\xi_i} = \begin{bmatrix} n_{ij}\rho u_j \\ n_{ij}\rho u_1 u_j + n_{i1}p \\ n_{ij}\rho u_2 u_j + n_{i2}p \\ n_{ij}\rho u_3 u_j + n_{i3}p \\ n_{ij}(E + p)u_j \\ n_{ij}\rho z_s u_j \end{bmatrix}$$

$$F_{v\xi_i} = \begin{bmatrix} 0 \\ n_{ij}\tau_{1j} \\ n_{ij}\tau_{2j} \\ n_{ij}\tau_{3j} \\ n_{ij}(\tau_{jk}u_k + q_j) \\ n_{ij}\rho D_s z_{s,j} \end{bmatrix}$$

$$E = e + 0.5\rho(u_1^2 + u_2^2 + u_3^2)$$

$$e = \sum_s \rho z_s (H_s + \Delta H_{f_s}) - p$$

$$\tau_{ij} = \mu(u_{i,j} + u_{j,i} - 2/3\delta_{ij}u_{m,m})$$

$$q_j = \kappa T_j + \sum_s \rho D_s h_s z_{s,j} \quad p = R_u T \sum_s \rho z_s \tag{2}$$

where z_s is the mole number density per unit mass of species s. The H_s and ΔH_{f_s} are the enthalpy and the heat of formation per mole of species s, respectively, and R_u is the universal gas constant. H_c is the chemical source term vector. The $(x_1, x_2, x_3) \equiv (x, y, z)$ and $(\xi_1, \xi_2, \xi_3) \equiv (\xi, \eta, \zeta)$ are Cartesian and curvilinear coordinate systems, respectively; $(\ )_{,i} \equiv \partial(\ )/\partial x_i$, V is the cell volume, and n_{ij} is the cell-interface normal vector. Finally, u_i, ρ, and p are the x_i velocity, the density, and the static pressure, respectively.

Computational Method

Discretization Method

The governing equations are discretized in a finite-volume formulation. The convective terms are evaluated using an upwind total variation diminishing (TVD) numerical flux based on Roe's approximate Riemann solver [12,13], considering the properties of the hyperbolic equations. The higher-order flux is constructed extrapolating the characteristics using two types of flux limiters [14]. The accuracy of the flux is third-order in smooth regions. A problem of ordinary TVD fluxes is that they fall into first order around the locations where the sign of the characteristics gradient changes. In such locations, this TVD numerical flux can be more dissipative than in smooth regions, but it remains second order and the order of the truncation error is still higher than the order of the viscous and diffusion terms. The viscous terms are evaluated with standard second-order difference formulae. The diffusion fluxes at the cell interfaces are modified so that the total mass is conserved [15]. The time integration method is the explicit Runge-Kutta multistage method. The second-order time integration is used.

Boundary Conditions

The surfaces of the nozzle tube are assumed to be slip walls. On the jet exit, the axial velocity is extrapolated, the total pressure and the total temperature are fixed to the values which realize a 1/7 power-law boundary layer when the exit pressure is the atmospheric pressure, and no artificial disturbance is imposed. At the outer boundaries, the non-reflection condition [16] is applied. At the initial state, the computational region is filled with still air. After the cold flowfield is established, heat is added for ignition.

Grid System

The grid system is rectangular. In this paper, the y-direction is the jet axial direction, the x- and z-directions are normal to the y-direction, and the origin is the jet exit center. The computational region is $-15D \le x, z \le 15D$ and $-3D \le y \le 20D$. The