Non-flamelet-like Premixed Flame Observed in a Simulation of Hydrogen Jet Lifted Flame

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1 Introduction

The advancement of computer power and computation technique has made it possible to simulate real-size combustion phenomena using detailed physical models. This kind of numerical simulation can be a strong scientific tool, that is, numerical experiment which is expected to bring novel information and knowledge on combustion science. The authors have succeeded in repoducing a hydrogen jet lifted flame by large scale numerical simulation with detailed chemistry and transport properties. The analysis of the obtained data shows that the flame is not a single-structured flame, but consits of three flame elements, ring-shaped leading edge flame, outer diffusion flame islands and an inner turbulent rich premixed flame. Among the three flame elements, the inner rich premixed flame is the most affected by the strong instability of the hydrogen jet and the effects of turbulence is so significant that the flame internal structure is disturbed[1-3]. In this paper, some attempts to understand the strongly turbulent rich premixed flame will be presented. The properties of the turbulent flame will be investigated mainly from the viewpoints of deviation from the laminar flamelet concept.

2 Numerical simulation

The flame configuration follows the experiment by Cheng et al.[4]. A hydrogen jet is injected into still air from a round nozzle whose diameter D is 2mm. The jet velocity is 680 m/sec, the Mach number is 0.54 and the Reynolds number based on the diameter is 13600. In the experiment, a lifted flame with the lift-off height of 7 D was observed.

The 9-species (H_2, O_2, OH, H_2O, H, O, H_2O_2, HO_2, N_2) and 17-reaction model by Westbrook [5] 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 are evaluated using the Lennard-Jones intermolecular potential model and Wilke's empirical rule. The enthalpy of each chemical species is derived from JANAF table.

The governing equations are the time-dependent compressible three-dimensional Navier-Stokes equations coupled with the conservation equations of chemical species. The governing equations are discretized by a finite-volume method. The convective terms are evaluated by third-order upwind numerical fluxes, viscous and diffusion terms by second order central difference formulae. The time integration is made by second-order Runge-Kutta method.

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The main grid system is a rectangular grid system and a cylindrical grid system is overlapped around the injection nozzle. The grid spacing is 0.05mm in the region of interest. This size is about 1/10 of the heat release layer width of the one-dimensional stoichiometric laminar premixed flame. The total grid number is about 200 million.

A stable lifted flame is obtained in the numerical simulation in the same way as in the experiment. The averaged lift-off height during the observation is around 6.5D. The lift-off height is slightly shorter than observation, but the agreement is fair considering the complexity of the problem and the difficulty in measurement and simulation.

The flame structure analysis based on Flame Index [6] ($\equiv \nabla Y_{H2} \cdot \nabla Y_{O2}$) shows that the lifted flame is not a single-structured flame but consists of three flame elements; 1. ring-shaped leading edge flame, 2. outer spot-like diffusion flame islands, 3. inner rich premixed flame. Figure 1 presents the structure of the simulated lifted flame. The instantaneous iso-surfaces of the hydrogen consumption rate at 10^4mol/sec/m^3 are shown with surface colors indicating the local combustion modes which can be defined using the Flame Index and the mixture fraction [7]. The surface colors, white, black and gray correspond to rich premixed, lean premixed and diffusive modes, respectively.

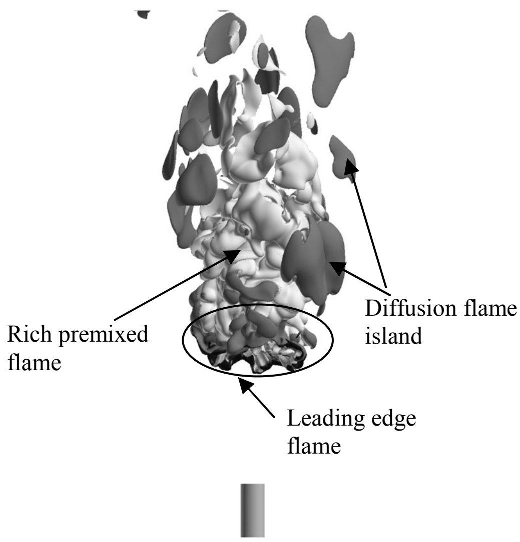

Figure 1: Flame structure, iso-surface of hydrogen consumption rate at 10^4mol/sec/m^3 (white: rich premixed, black: lean premixed, gray: diffusive).

3 Vigorously turbulent inner rich premixed flame

The Kelvin-Helmholtz (K-H) instability of the hydrogen jet produces the turbulence in the lifted flame. Figure 2 shows the turbulent hydrogen jet which has a vigorously turbulent and strongly three-dimensional feature. Very small structures produced by K-H instability are observed in the upstream unburnt region. As going downstream into the burnt region, the very small structures are suppresed by the large diffusivity of hot burnt gas, and only rather large structures remain.

The effects of vigorous turbulence appear the most remarkably in the inner rich premixed flame among the three flame elements. The turbulence produces some unusual aspects of the inner rich premixed flame, for example, the heat release layer looks largely deviated from the fuel consumption layer as shown in Fig.3, although the two layers are expected to be almost parallel in laminar flames [1]. The turbulence affects also the outer diffusion flame islands. The vigorously turbulent behavior of the inner rich premixed flame plays an important role in the formation process of the spot-like shape of the outer diffusion flame islands [3].

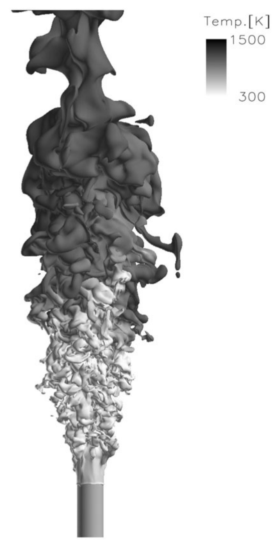

Figure 2: Turbulent hydrogen jet . Iso-surface of hydrogen mole fraction at 60% with surface color corresponding to the temperature.

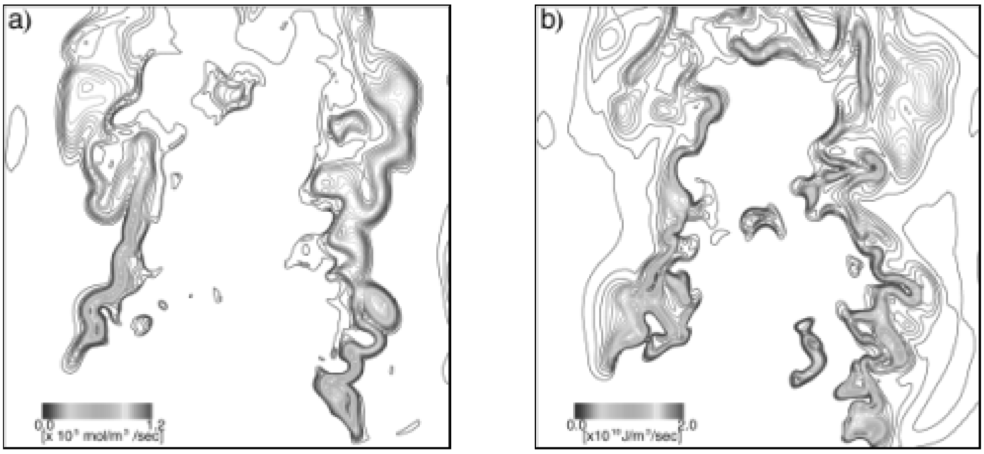

Figure 3: Deviation of heat release layer from hydrogen consumption layer in the inner rich premixed flame, a): hydrogen consumption rate b): heat release rate.

The properties of the vigorously turbulent flame are investigated from the viewpoints of difference from the laminar flamelet concept in the following.

One of the most important aspects of the laminar flamelet is the balance between fuel supply by molecular diffusion and fuel consumption by reactions in the reaction zone. Figure 3 shows the balance between the two terms on the iso-surface in Fig.1. Two terms are nearly in balance in gray region, molecular diffusion largely exceeds in white region and consumption largely exceeds in black region. In the large part of the diffusion flame islands, the two terms are in balance. On the other hand, in most part of the inner rich premixed flame, one term largely exceeds the other. It indicates that the necessary condition of the laminar flamelet concept is not satisfied in most part of the inner rich premixed flame.

The second viewpoint is the sensitivity of the fuel consumption on the respective transport terms. If the combustion is controlled by the molecular diffusion as assumed in the laminar flame concept, the change of the fuel consumption should follow the change of the molecular diffusion of the fuel. When we assume that the fuel consumption rate depends on the convections in flame-normal and flame-tangential directions and molecular diffusions in flame-normal and flame-tangential directions, the differential equation may be written as,

$$dS = a_1 dC^n + a_2 dC^t + a_3 dD^n + a_4 dD^t \ ,$$

where S, C, D are the chemical reaction, convection and diffusion terms of the conservation equation of hydrogen, respectively, and subscripts n and t denote flame-normal and flame-tangential directions. The coefficients a_1-a_4 can be calculated by using the four neighboring points on the flame surface. If the fuel consumption is completely controlled by fuel molecular diffusion in the flame normal direction, a_1=a_2=a_4=0 and a_3=-1. The coefficients are estimated on the iso-surface shown in Fig.1. On the inner premixed flames, no coefficients are dominant and a_3 is largely different from -1, while a_3 is dominant and

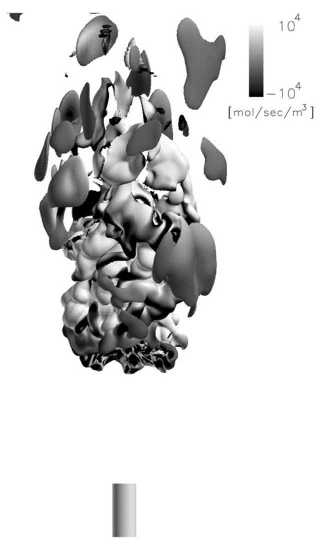

Figure 4: Balance between fuel supply by molecular diffusion and fuel consumption by combustion reactions, gray: almost in balance, white: molecular diffusion exceeds, black: consumption exceeds.

nearly -1 on the outer diffusion flames. The result indicates that it is not easy to describe the fuel consumption in the inner turbulent premixed flame by the fuel molecular diffusion into the reaction layer.

To see the location of the flame in the conventional turbulent premixed flame regime diagram, the turbulence and flame scales have been estimated at a point in the inner rich premixed flame, where the deviation of heat release layer from the fuel consumption layer is large. The analysis shows that the turbulence eddy size varies from 0.03mm to 3mm, and the reaction zone thickness is about 1mm. It indicates that turbulent eddies can easily penetrate into the reaction zones to modify the internal structure of the flame. In Borghi's diagram [8], the premixed combustion at the measured point is categorized into the well-stirred reactors regime (v'/S_L=33, l/l_F =2).

As shown above, it is clear that the conventional laminar flamelet concept is not applicable to the inner rich premixed flame. More detailed analysis of the obtained numerical data must be required to make clear this structure.

4 Summary

The detailed numerical simulation of a hydrogen jet lifted flame predicts that vigorously turbulent flame exists in the inner side of the flame. Small turbulent eddies can penetrate into the reaction zone and modify the flame internal structure, therefore, the conventional laminar flamelet concept is not applicable to the flame.

Further investigations are required to understand the flame structure. For the purpose, development of novel analytical concepts and principles is indispensable.

References

[1] Mizobuchi, Y., Tachibana, S., Shinjo, J., Ogawa, S., and Takeno, T., Proc. Combust. Inst. 29, 2002, pp. 2009-2015.

[2] Westbrook, C. K., Mizobuchi, Y., Poinsot, T. J., Smith, P. J. and Warnatz, J., Proc. Combust. Inst. 30, 2004, pp. 125-157.

[3] Mizobuchi, Y., Shinjo, J., Ogawa, S. and Takeno, T., Proc. Combust. Inst. 30, 2004, pp. 611-619.

[4] Cheng, T. S., Wehrmeyer, J. A. and Pitz, R. W., Combustion and Flame, 91, 1992, pp. 323-345.

[5] Westbrook,C.K. Combustion Science and Technology, 29, 1982, pp.67-81.

[6] Yamashita, H., Shimada, M. and Takeno, T., Twenty-sixth Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1996, pp. 27-34.

[7] R. W. Bilger, R. W., Proc. Combust. Inst., 22, 1988, pp. 475-488.

[8] Borghi, R., Recent Advances in the Aerospace Science, Plenum, New York, 1985, pp. 117-138.