Numerical Analysis on Stabilization of a Lifted Flame

Yasuhiro Mizobuchi, Junji Shinjo and Shigeru Tachibana

CFD Technology Center National Aerospace Laboratory of Japan 7-44-1 Jindaijihigashi, Chofu, Tokyo 182-8522, Japan

A hydrogen lifted flame is numerically analyzed by DNS approach. The investigations are mainly focused on its structure and stabilization mechanism. The diameter of hydrogen injector is 2mm and the injection velocity is 680 m/sec. The time dependent 3-D simulation was made with a full chemical kinetics and rigorous transport properties. 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. an 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 is stabilized outside the turbulent jet and has a triple flame like structure with the normalized flame index around unity, indicating that the incoming flow almost balances with the laminar burning velocity. The lifted flame is strongly stabilized by the stable leading edge flame.

1. INTRODUCTION

To develop a novel premixed combustor system which realizes high efficiency and low pollutant emission, detailed investigations on the flame behavior around the flame stabilization locations are indispensable. The understanding of the flame stabilization mechanism will lead to the extension of the flammability limit, which is expected to be an effective means to achieve the requirements. In practical combustors, when optimized to operate beyond the traditional flammability limit, the mixture fraction distribution should be controlled to be appropriately stratified, not perfectly premixed or perfectly non-premixed, but partially premixed. Hence, the combustion flowfield of partially premixed flame should be observed in detail by experimental or numerical approach and the mechanisms of flame holding, blow-off and extinction around the flame stabilization locations should be investigated.

One representative partially premixed flame configuration is lifted flame. Lifted flame is a fundamental flame configuration, but it contains combustion in stratified medium, and therefore it is an important research subject from the practical point of view, as well as from the fundamental point of view. The major research subjects on lifted flame have been the flame structure and the stabilization of lifted flame, and they have been investigated enthusiastically from the viewpoints of the flamelet extinction[1] and the triple flame structure[2, 3, 4, 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 DNS (Direct Numerical Simulation) approach and succeeded to capture the lifted flame solution[6]. The timedependent three-dimensional simulations have been made with a full chemical kinetics and rigorous transport properties. The computation with about 23 million grid points has been conducted using the vector parallel computer Numerical Wind Tunnel (NWT) at National Aerospace Laboratory of Japan (NAL).

From the observations of simulated complicated combustion flow field and short-term ($\simeq 0.1$ msec) 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 using the normalized flame index[7] and three flame elements are introduced. Then stabilization at the flame base is investigated.

The analysis methods developed and some knowledge obtained throughout this work on a hydrogen flame are general and they will contribute to the numerical analysis of other fuel flames such as a methane flame.

2. FLAME CONFIGURATIONS

The flame configurations are subject to the experiment by Cheng et al.[8]. 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. A lifted flame was observed in the experiment and the lift-off height was 7 diameters.

3. COMPUTATIONAL METHOD

3.1 Computational Model

A detailed chemistry for hydrogen/air system is used. 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[9] is employed. The air is assumed to be composed of 22% O_2 and 78% N_2 in volume. The diffusion of chemical species is evaluated using Fick's law with binary diffusion coefficients. The transport coefficients of each chemical species are estimated using the Lennard-Jones intermolecular potential model. The enthalpy of each chemical species is derived from the JANAF thermochemical table[10]. No turbulence model is used.

3.2 Discretization of government equations

The governing equations are the compressible three-dimensional Navier-Stokes equations coupled with the conservation equations of chemical species. The equation of total mass conservation is solved additionally. The governing equations are discretized in a finite-volume formulation. The convective terms are evaluated using a TVD numerical flux based on Roe's approximate Riemann solver[11, 12]. The higher-order flux is constructed extrapolating the characteristics using two types of flux limiters[13]. The accuracy of this flux is third-order in smooth regions and second-order around regions where the sign of characteristics gradient changes. The viscous terms are evaluated with standard second-order difference formulae. The diffusion fluxes are evaluated by Fick's law with binary diffusion coefficients and, therefore the diffusion fluxes are modified so that the total mass is conserved[14]. The time integration method is the explicit Runge-Kutta multi-stage method. The second order time integration is used.

The surfaces of the nozzle tube are assumed to be slip walls. On the jet exit the y-direction 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. No artificial disturbance is imposed. At the outer boundaries the non-reflection condition[15] is applied. After the cold flowfield is established, heat is added for ignition.

3.3 Grid system

To conduct DNS of turbulent combustion flow, we have to resolve the turbulent scale and the combustion scale. The turbulent scale is the Kolmogorov scale and it is recently reported that the smallest eddy size to be resolved is about 10 times as large as the Kolmogorov scale[16]. The combustion scale is the inner reaction layer width that is about 1/10 of the flame thickness. One-dimensional laminar premixed flame simulation shows that the inner layer width is about 0.5mm when the equivalence ratio of the hydrogen-air mixture is 1.0.

The grid system is rectangular. The computational region is 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 grid spacing is 0.05mm in $-1.25D \le x, z \le 1.25D$, $0 \le y \le 8D$. This size is 2.5 times as large as the Kolmogorov scale measured in the experiment around the ignition point and about 1/10 of the inner layer width. The grid spacing is coarser as the distance from the above mentioned region is longer. The total grid number is about 23 million.

4. RESULTS AND DISCUSSION

The plateau state is obtained about 2msec after the ignition and the computation time is about 4000 hours. A lifted flame is obtained in the numerical simulation in the same way as in the experiment as shown in fig.1. The averaged lift-off height during the observation is around 5.5 diameters. The simulated lift-off height is slightly shorter than the experimental one, but this agreement is fair considering the difficulty of the problem.

4.1 Flame structure analysis by normalized flame index

The flame structure is analyzed using the flame index (F.I.)[7]. It is defined as,

$$F.I. = \nabla Y_{H_2} \cdot \nabla Y_{O_2}, \tag{1}$$

where Y_s is the mass fraction of chemical species s. The flame is premixed when F.I. is positive and diffusion when F.I. is negative. The positive F.I. is normalized by the F.I. of the laminar premixed flame at corresponding local mixture fraction. The negative F.I. is normalized by the F.I. at the extinction limit of the counter diffusion flame. A very complicated three-dimensional flame structure is visualized by iso-surfaces of the normalized flame index (N.F.I.) in fig.2. The iso-surfaces at 1.0 and -0.02 are painted yellow and green, respectively. The N.F.I. is set to zero where the temperature is less than 600K for better observation. Turbulent premixed flames are observed in the inner side and diffusion flame islands in the outer side. The strong turbulence in the inner premixed flame is caused by the instability of the hydrogen jet.



Figure 1: Instantaneous iso-surface of temperature at 1000K with hydrogen density on the surface.

Figure 2: Instantaneous iso-surface of N.F.I., yellow : premixed flame, N.F.I.= 1.0, green : diffusion flame, N.F.I.= -0.02.

The instantaneous N.F.I. distribution in the x - y plane is presented in fig. 3, and the zoom-up view around the leading edge is also shown. The positive iso-level contours are drawn with solid lines from 0.4 to 10.0 by 0.4 and the negative contours are drawn with dashed lines from -0.02 to -0.1 by 0.02. The stoichiometric mixture fraction ($z_{st}=0.02957$) lines are drawn with thick black lines. The inner premixed flame is rich and vigorously turbulent, and the outer diffusion flame islands are aligned along the stoichiometric lines. The leading edge flame is composed of, rich premixed flame, diffusion flame and lean premixed flame, and has a triple flame like structure.

Figures 4 a) and b) show the time traces of the axial velocity and heat release rate, respectively, at the location A and B in fig. 3. At the location B, the velocity and the heat release are strongly unsteady and the fluctuations are large. On the other hand at the location A, the flowfield is very calm and laminar and the heat release is very stable. As is represented by the location A, the leading edge flame is located around the stoichiometric line, that is, outside the turbulent jet, and therefore the velocity is small and the flow is almost laminar.

From the above investigation, it can be concluded that the lifted flame consists of a stable leading edge flame, an inner turbulent premixed flame and outer floating diffusion flame islands.



Figure 3: Instantaneous distribution of N.F.I. in x-y plane. Positive iso-lines are drawn with solid lines, negative with dashed lines and stoichiometric mixture fraction iso-lines with thick lines.



Figure 4: Time trace of a):axial velocity and b):heat release rate at the locations A and B in fig. 3.

4.2 Flame stabilization

The location A in fig.3 is one of the most stable locations during the observation. The N.F.I. is about unity around the location A, which indicates that the incoming flow almost balances with the laminar burning velocity. This is because the flame index is proportional to the laminar burning velocity. In fact, the axial velocity at the location A varies from -2 to 10 m/sec as shown in fig.4 a) and the average is about 3 m/sec, while the laminar burning velocity corresponding to the local mixture fraction is calculated to be about 2 m/sec.

Figure 5 shows the three-dimensional view of the leading edge flame from below. The isosurfaces of the hydrogen consumption rate at 10^4 mol/m³/sec are drawn and the colors on the surfaces correspond to the flame configurations. The rich premixed flame regions, where N.F.I. > 0 and the mixture fraction $z > z_{st}$, are painted red, the lean premixed flame regions, where N.F.I. > 0 and $z < z_{st}$, are blue and the diffusion flame regions, where N.F.I. < 0, are green. The leading edge flame of a ring shape is strongly three-dimensional and has a large variation in the circumferential direction. In most part of the upstream end of the leading edge flame, the flame is lean premixed flame. Figure 6 shows the instantaneous axial velocity on the lean premixed flame surfaces of N.F.I. of a) : 0.5, b) : 1.0 and c) : 5.0. In the lean premixed flame of the leading edge flame, N.F.I. is not so large and is of order of unity, and the axial velocity is so small as to balance with the burning velocity as observed in the location A. This stable lean premixed flame stabilizes the leading edge flame. The structure of the leading edge flame is strongly three-dimensional and slowly varies with time. At some locations, the upstream end is not lean premixed flame and the triple flame like structure is broken. We need more detailed analysis based on long-term and three-dimensional observation to understand the stabilization mechanism of the leading edge flame.





Figure 5: Instantaneous three-dimensional view of leading edge flame from below. Hydrogen consumption rate iso-surfaces at 10^4 mol/m³/sec are drawn and the surface colors correspond to the flame configurations, red : rich premixed, blue : lean premixed, green : diffusion.

Figure 6: Instantaneous axial velocity distribution on the lean premixed flame of N.F.I. of a) : 0.5, b) : 1.0, c) : 5.0, color level red corresponds to axial velocity $v_{ax} \geq 10$ m/sec and blue to $v_{ax} \leq -10$ m/sec.

The inner premixed turbulent flame is vigorously turbulent and very large N.F.I. is observed in the flame as shown in fig.3. In such locations the flame is going toward extinction due to excess gas supply by diffusion, and therefore the inner turbulent premixed flame is very unstable in itself. This very unstable turbulent premixed flame is strongly stabilized by the stable leading edge flame.

The outer floating diffusion flame islands are not stabilized at the fixed positions but flow slowly downstream along the stoichiometric plane. Figure 7 shows the production process of the diffusion flame islands. The hydrogen consumption rate iso-surfaces at 10^4 mol/m^3 /sec are drawn with the N.F.I. distribution on the surfaces at sequential time stages ($\Delta t = 30 \text{ msec}$). The light blue regions correspond to positive N.F.I., that is, to the premixed flame and the regions from green to red correspond to the diffusion flame. Due to the vigorous turbulent motion, the hydrogen consumption layer of the inner premixed flame reaches the stoichiometric plane at some locations, where the combustion is activated. After that, break-off of the inner premixed flames occurs and then diffusion flame islands are detached from the inner premixed flames and flow downstream.

As discussed above, the entire stabilization of the lifted flame is achieved by the stable leading edge flame. The leading edge flame stabilizes the inner turbulent premixed, and the inner turbulent premixed flame produces the floating diffusion flame islands.

5. CONCLUSION

A hydrogen lifted flame is numerically simulated by DNS approach with a full chemical kinetics and rigorous transport properties. The results are analyzed by N.F.I. and it is shown that the lifted flame is not a single flame but a complicated flame consisting of a stable leading edge flame, an inner turbulent premixed flame and floating diffusion flame islands.

The leading edge flame is strongly stable because it is located outside the jet. It has a triple flame like structure and the stabilization is mainly maintained by the lean premixed flame where N.F.I. is of order of unity. The inner vigorously turbulent premixed flame is stabilized by the stable leading edge flame. The floating diffusion flame islands are produced by the vigorous turbulent motion of the inner turbulent premixed flame.

The structure of the lifted flame is strongly three-dimensional, and some fluid motions have

larger time scales than the observation term of this work. Further investigation based on a long-term and three-dimensional observation is needed to understand the detailed mechanism of the flame stabilization.



Figure 7: Production of diffusion flame islands. Hydrogen consumption rate iso-surfaces at $10^4 \text{ mol/m}^3/\text{sec}$ are drawn with distribution of N.F.I. on the surfaces at sequential time stages in a), b) and c), with time interval of 30 μ sec.

REFERENCES

- [1] Nobert Peters and Forman A. Williams. AIAA Journal, 21(3):423–429, 1983.
- [2] P. N. Kiori, B. Rogg, K. N. C. Bray, and A. Liñán. Combusiton and Flame, 95:276–290, 1993.
- [3] G. R. Ruetsch and L. Vervisch. Physics of Fluids, 7(6):1447–1454, 1995.
- [4] V. Favier and L. Vervisch. In Proceedings of Twenty-Seventh Symposium (International) on Combustion, 1239–1245, Pittsburgh, 1998.
- [5] Luc Vervisch and Thierry Poinsot. Annual Review of Fluid Mechanics, 30:655–691, 1998.
- [6] Y. Mizobuchi, S. Tachibana, J. Shinjo, S. Ogawa, and R. Takaki. IUTAM Symposium on Turbulent Mixing and Combustion to be published, 2001.
- [7] H. Yamashita, M. Shimada, and T. Takeno. Proceedings of Twenty-Sixth Symposium (International) on Combustion, 27–34, Pittsburgh, 1996.
- [8] T. S. Cheng, J. A. Wehrmeyer, and R. W. Pitz. Combustion and Flame, 91:323–345, 1992.
- [9] C. K. Westbrook. Combustion Science and Technology, 29:67–81, 1982.
- [10] JANAF. JANAF Thermochemical Tables. 1965.
- [11] P.L. Roe. Journal of Computational Physics, 43:357–372, 1981.
- [12] Y. Wada, S. Ogawa, and T. Ishiguro. AIAA paper 89-0202, 1989.
- [13] Y. Wada. PhD thesis, the University of Tokyo, 1995.
- [14] Y. Mizobuchi and S. Ogawa. AIAA paper 2000-0184, 2000.
- [15] K. W. Thompson. Journal of Computational Physics, 68:1–24, 1987.
- [16] P. Moin and K. Mahesh. Annual Review of Fluid Mechanics, 30:539–578, 1998.