

Analysis of a Hydrogen Jet Lifted Flame by 3-D Numerical Simulation

with Detailed Chemistry and Transport Properties

Yasuhiro Mizobuchi¹, Junji Shinjo¹, Shigeru Tachibana¹, Satoru Ogawa¹ and Tadao Takeno²

¹CFD Technology Center, National Aerospace Laboratory of Japan
7-44-1 Jindaiji-Higashi, Chofu, Tokyo 182-8522, Japan
E-mail : mizo@nal.go.jp

²Department of Mechanical Engineering, Meijo University
1-501 Shiogamaguchi, Tempaku-ku, Nagoya 468-8502, Japan

Key Words : 3-D Simulation, Jet Lifted Flame, Flame Structure, DNS

1. INTRODUCTION

Numerical simulation is now a very strong tool for combustion research. Development of computer resource and computational technique has enabled us to conduct three-dimensional combustion simulations that resolve the internal structures of the thin reaction layers in flames with detailed chemistry and rigorous transport properties. Some findings from such kinds of simulations will contribute to the understanding of novel combustion phenomena that have not been observed in experiments, and some should be used for the development of combustion modeling. Hence, the importance of the analysis of the obtained huge data is getting larger and larger with the progress of numerical simulations.

The authors succeeded to capture a hydrogen/air turbulent jet lifted flame by DNS (Direct Numerical Simulation) approach[1]. The time-dependent 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) which was run till June 2002 at National Aerospace Laboratory (NAL) of Japan. The obtained huge data has been analyzed mainly based on the concept of the laminar flame theory. In this paper, the structure of the lifted flame is investigated first and then the characteristics of the flame elements are discussed.

2. FLAME CONFIGURATIONS

The flame configuration followed the experiment by Cheng et al.[2]. 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 diameters was observed.

3. COMPUTATIONAL MODEL AND GOVERNING EQUATIONS

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[3] is employed. The elementary reactions are listed in Table 1. 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[4] and Wilke's empirical rule[5]. The enthalpy of each chemical species is derived from JANAF[6].

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. The governing equations are discretized by a finite-volume method. For the details, see ref. [7].

4. COMPUTATIONAL GRID

The grid system is rectangular. The grid spacing is 0.05mm around the jet core. This size is 2.5times as large as the Kolmogorov scale measured in the experiment around the ignition point, and is about 1/10 of the heat release layer width of the one-dimensional stoichiometric laminar premixed flame. The grid number is about 23 million.

5. RESULTS AND DISCUSSION

A stable lifted flame is obtained in the numerical simulation in the same way as in the experiment. The iso-surface of temperature at 1000 K is shown in Fig.1. The averaged lift-off height during the observation is around 11mm. The simulated lift-off height is slightly shorter than the experimental one, but this agreement is fair considering the difficulty of the problem.

5.1. Structure of the lifted flame

An useful variable to analyze the flame structure is flame index. It is defined as[8],

$$\text{F.I.} = \nabla Y_{\text{H}_2} \cdot \nabla Y_{\text{O}_2}, \quad (1)$$

where Y_s is the mass fraction of chemical species s . The flame is a premixed flame when the F.I. is positive and a diffusion flame when the F.I. is negative.

Figure 2 presents the instantaneous iso-surface of the hydrogen consumption rate at 10^4 mol/sec/m^3 . The surface color corresponds to the local combustion mode which can be defined using the flame index and the mixture fraction [9]. The surface colors red, blue and green correspond to rich premixed, lean premixed and diffusion flames, respectively. One can see that the lifted flame is not a single flame but consists of three flame elements; 1. a leading edge flame, 2. an inner rich premixed flame, 3. outer diffusion flame islands. The observation of the unsteady flame behavior shows the following features of the flame elements. The leading edge flame, which is composed of rich/lean premixed flames and diffusion flames, is stable to stabilize the global system of the lifted flame. The inner rich premixed flame is vigorously turbulent. The outer diffusion flames are not stabilized at the fixed positions but flow slowly downstream along the stoichiometric plane.

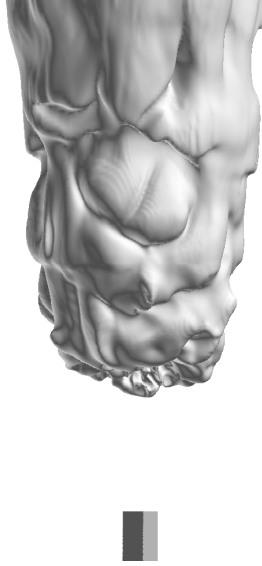


Figure 1: Instantaneous iso-surface of temperature at 1000K.

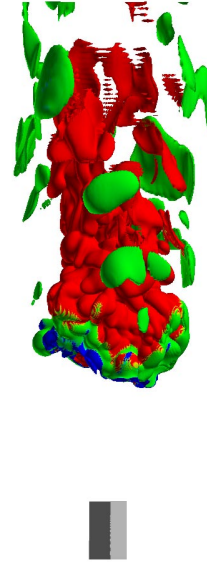


Figure 2: Global structure of the lifted flame. Instantaneous iso-surfaces of hydrogen consumption rate at 10^4 mol/sec/m^3 are drawn where the surface color corresponds to the combustion mode, red:rich premixed, blue:lean premixed, green:diffusion.

5.2 Effects of turbulence on the flame

The inner rich premixed flame is affected most by the strong instability of the hydrogen jet. One of the interesting phenomena observed in the inner rich premixed flame is deviation of the heat release layer from the hydrogen consumption layer. Figure 3 a) and b) show the instantaneous distributions of hydrogen consumption rate and heat release rate, respectively, in a cutting plane and in the upper half of the figures, the deviation is remarkable. The displacement is strongly distributed and modified and largely different from that observed in laminar flames.

The time scale analysis is conducted to investigate the internal structure modification. In the turbulent premixed flames, the time scale of turbulent convection τ_f is quite small and the Fourier analysis of the mixture fraction fluctuation shows that τ_f is from 0.02 to 0.05 msec in the region of large deviation. The reaction time scale in the flame can be defined as $\tau_r = \Delta x / S_L$, where Δx is the distance between the peak locations of hydrogen consumption rate and heat release rate in one-dimensional premixed flame and S_L is the corresponding laminar burning velocity. This time scale can be estimated using the local mixture fraction. Around the stoichiometric condition τ_r is the smallest and it becomes larger abruptly as the mixture becomes rich or lean. In the regions where the deviation is remarkable, the mixture is very rich and the mixture fraction is from 0.08 to 0.12, which corresponds to τ_r from 0.05 to 0.15msec. The two time scales are of the same order, and that τ_f is smaller than τ_r . Hence, the kinetics in the reaction layers can be easily disturbed by turbulent convection and the deviation is produced.

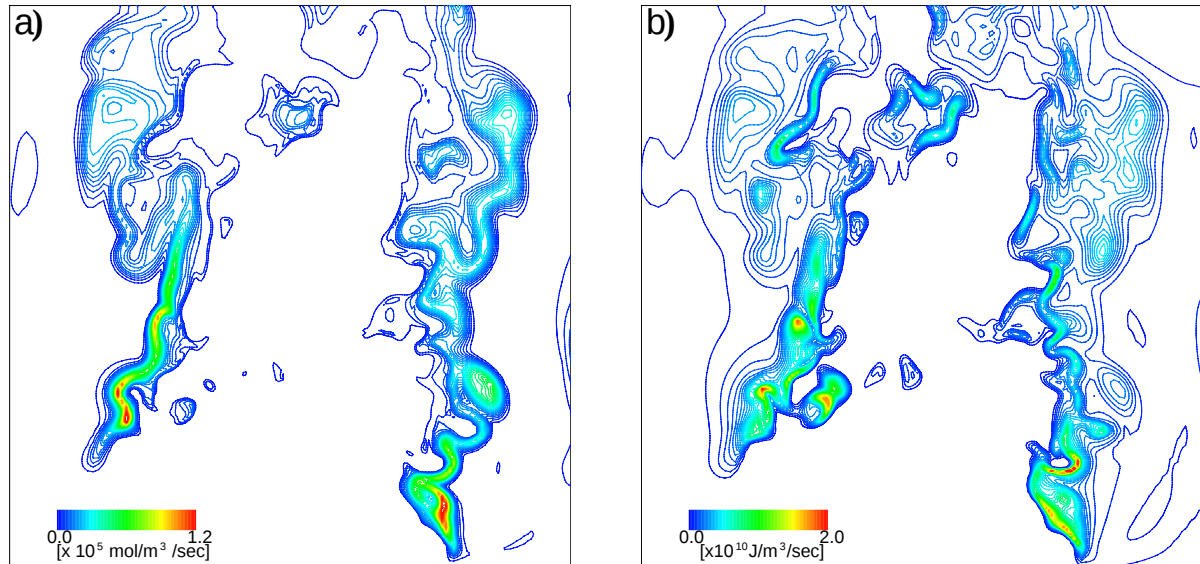


Figure 3: Deviation of heat release layer from hydrogen consumption layer in the inner turbulent rich premixed flame, a) : hydrogen consumption rate b) : heat release rate.

6. CONCLUSIONS

Various aspects of a hydrogen jet lifted flame have been revealed by three-dimensional DNS and its data analysis. This kind of three-dimensional DNS studies are very useful to study various very complicated flame structures.

ACKNOWLEDGMENTS

This research was carried out as a research activity at the Center for Smart Control of Turbulence funded by MEXT (Ministry of Education, Culture, Sports, Science and Technology) of Japan.

REFERENCES

- [1]. Y. Mizobuchi et al., *IUTAM Symposium on Turbulent Mixing and Combustion*, pages 337–345, 2002.
- [2]. T. S. Cheng, J. A. Wehrmeyer, and R. W. Pitz, *Combustion and Flame*, 91:323–345, 1992.
- [3]. C. K. Westbrook, *Combustion Science and Technology*, 29:67–81, 1982.
- [4]. S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases*, 1970.
- [5]. C. R. Wilke, *Journal of Chemical Physics*, 18(4):517–519, 1950.
- [6]. D. R. Stull et al, *JANAF Thermochemical Tables*, 1965.
- [7]. Y. Mizobuchi and S. Ogawa, *AIAA paper 2000-0184*, 2000.
- [8]. H. Yamashita, M. Shimada, and T. Takeno, *Proc. 26th Symp.(Int.) on Combustion*, pages 27–34, 1996.
- [9]. R. W. Bilger, *Proc. 22nd Symp.(Int.) on Combustion*, pages 475–488, 1988.