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A numerical study on the formation of diffusion flame islands in a turbulent hydrogen jet lifted flame

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Abstract

This paper presents a numerical study on the formation of diffusion flame islands in a hydrogen jet lifted flame. A real size hydrogen jet lifted flame is numerically simulated by the DNS approach over a period of about 0.5 ms. The diameter of hydrogen injector is 2 mm, and the injection velocity is 680 m/s. The lifted flame is composed of a stable leading edge flame, a vigorously turbulent inner rich premixed flame, and a number of outer diffusion flame islands. The relatively long-term observation makes it possible to understand in detail the time-dependent flame behavior in rather large time scales, which are as large as the time scale of the leading edge flame unsteadiness. From the observation, the following three findings are obtained concerning the formation of diffusion flame islands. (1) A thin oxygen diffusion layer is developed along the outer boundary of the lifted flame, where the diffusion flame islands burn in a rather flat shape. (2) When a diffusion flame island comes into contact with the fluctuating inner rich premixed flame, combustion is intensified due to an increase in the hydrogen supply by molecular diffusion. This process also works for the production of the diffusion flame islands in the oxygen diffusion layer. (3) When a large unburned gas volume penetrates into the leading edge flame, the structure of the leading edge flame changes. In this transformation process, a diffusion flame island comes near the leading edge flame. The local deficiency of oxygen plays an important role in this production process.

Keywords: Jet lifted flame; Flame island; DNS

1. Introduction

Numerical simulation is becoming a more and more powerful tool in combustion research. The recent remarkable development of computer resources, as well as computational techniques, has enabled us to conduct a time-dependent three-dimensional simulation of actual size flame that accurately resolves the detailed internal structures of thin reaction layers with detailed chemical models and rigorous transport properties. The significance of this kind of huge numerical simulation lies in finding novel combustion phenomena and understanding their mechanisms by analysis, as well as in contributing to combustion model construction.

The authors succeeded in capturing a hydrogen/air turbulent jet lifted flame by the direct numerical simulation (DNS) approach [1]. The motivation lay in the understanding of the structure and the stabilization mechanism of the jet lifted flame that has been investigated by various

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approaches [2–6]. The time-dependent three-dimensional simulations were made with full chemical kinetics and rigorous transport properties. The computation with about 23 million grid points was conducted to resolve the turbulent small scale and flame internal structure. They showed that the flame is not a single flame, but is composed of three flame elements: the stable leading edge flame, turbulent rich premixed flame, and a number of island-like diffusion flames. From the short-term ($\simeq$0.1 ms) observation of the unsteady flame behavior, interesting aspects of the flame elements were revealed.

The data acquisition has been successively conducted using the symmetric multi-processor (SMP) cluster system named Central Numerical Simulation System (CeNSS) at the Institute of Space Technology and Aeronautics, Japan Aerospace Exploration Agency (JAXA). A longer-term observation has been achieved over a period of about 0.5 ms. During the observation, the lifted flame is stabilized, and several vortices pass through the leading edge flame. Then, it has become possible to analyze in detail the unsteady flame behaviors that take place in the time scale of the leading edge flame unsteadiness, which is much larger than that of the turbulent jet instability.

For the statistical post-processing analysis leading to combustion modeling, we need to develop some new methodology, especially when we tackle complicated and novel flame configurations. So we adopt the following strategy. The global structure should be understood first, and then a detailed process of the respective flame elements is investigated to understand the physics and chemistry of the process. Finally, we will challenge to develop a numerical model to describe the jet flame. In the last paper[1], we understand about the global structure of the lifted flame. However, a detailed process of the respective flame elements has not yet been well understood. One of the flame elements peculiar to this turbulent jet lifted flame is the island-like diffusion flame structure, which is typically observed along the outer boundary of the lifted flame. The authors named these "diffusion flame islands" and briefly discussed their production process. The present longer-term simulation provides more detailed information and more opportunities to observe the production/intensification events of the diffusion flame islands. In this study, the new findings on the formation of the diffusion flame islands are presented and discussed.

2. Lifted flame configuration

The configuration of the hydrogen jet lifted flame follows 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 the lift-off height of 7 diameters was observed.

3. Computational method

The 9-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 thermal and transport properties of the gas mixture are vigorously calculated [9–11]. 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 discretization is based on a finite volume method. Third-order upwind numerical flux [12] based on Roe's scheme [13] is used for convection terms. The higher-order flux is constructed extrapolating the characteristics using two types of flux limiters. The accuracy of this flux is third-order in smooth regions and remains second-order around regions where the sign of characteristic gradient changes. The molecular diffusion flux is modified so that the total mass conservation is satisfied. Time integration method is the second-order Runge–Kutta method. For details, see [14]. The nozzle tube is assumed to be square, and the surface is assumed to be a slip wall. On the jet exit, the total pressure and the total temperature are fixed so that a fully turbulent pipe flow profile is reproduced when the exit pressure is atmospheric. The outer boundaries are non-reflecting boundaries [15]. The grid system is rectangular. The grid spacing around the jet core region is 0.05 mm, which is about 1/10 of the hydrogen consumption layer thickness of a stoichiometric hydrogen/air premixed flame calculated by PREMIX [16]. The total grid number is about 23 million.

4. Results and discussion

The global structure of the lifted flame is clearly illustrated by use of the flame index [17]. Flame index (F.I.) is defined as

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

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. Figure 1 presents the instantaneous flame structure obtained by the numerical simulation and to be studied in this paper. The iso-surfaces of the hydrogen consumption rate at 10^4 mol/s/m^3 are drawn, where the surface color corresponds to the local combustion mode that is determined by the flame index and the mixture fraction in Bilger's definition [18].

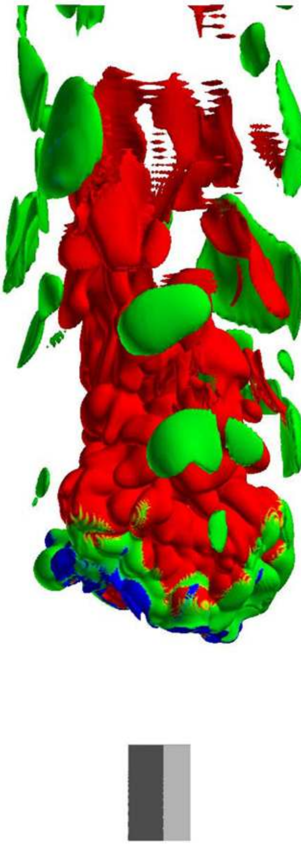

Fig. 1. Global structure of the hydrogen jet lifted flame. Instantaneous iso-surface of hydrogen consumption rate at 10^4 mol/s/m^3. Surface color shows the combustion mode, red: rich premixed, blue: lean premixed, and green: diffusion.

The red, blue, and green surfaces correspond to rich premixed, lean premixed, and diffusion flames, respectively. One can see the three flame elements; (1) a leading edge flame, (2) an inner rich premixed flame, and (3) outer diffusion flame islands. The averaged lift-off height is about 5.5*D*, which is slightly shorter than the experimental observation, but this fair agreement in the lift-off height implies that the simulation captures most of the physics that take place in the jet lifted flame. Figure 2 is the two-dimensional view of the hydrogen consumption rate distribution at that moment. The iso-lines of hydrogen consumption rate are drawn with an interval of 5000 mol/m^3/s. Based on the sign of the flame index, the premixed mode consumption is drawn with solid lines and diffusive with dashed. The thick black lines are the stoichiometric mixture fraction (= 0.02957) lines. Most of the hydrogen consumption takes place in rich and lean premixed branches of the leading edge flame, and diffusive combustion is not so intense.

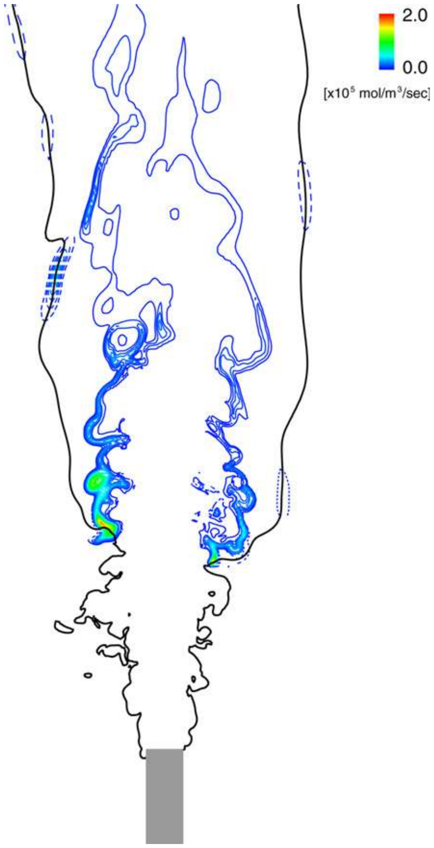

Fig. 2. Instantaneous distribution of hydrogen consumption rate in a cutting surface that includes the jet centerline. Premixed and diffusive consumption are drawn with solid and dashed lines, respectively, with an interval of 5000 mol/s/m^3. Stoichiometric mixture fraction lines are drawn with thick black lines.

In this study, the diffusion flame islands are of interest, and three major findings will be discussed about the formation of diffusion flame islands. One is the thin oxygen diffusion layer where the diffusion flame islands can exist. The other two are the intensification/production processes of the diffusion flame islands by the unsteady behaviors of the inner rich premixed flame and by the leading edge flame.

4.1. Thin oxygen diffusion layer

The instantaneous two-dimensional distribution of the oxygen mass fraction is shown in Fig. 3. The stoichiometric line is drawn with thick black lines, and diffusion flame islands are illustrated in light gray as regions where the hydrogen consumption rate is larger than 5000 mol/s/m^3. The oxygen, which has been entrained into the jet flow upstream of the flame, is consumed at the leading edge flame, and therefore the oxygen

Fig. 3. Instantaneous distribution of oxygen mass fraction. The iso-lines are drawn from 0.005 to 0.25 with an interval of 0.005. Stoichiometric mixture fraction lines are drawn with thick black lines. Diffusion flame islands (hydrogen consumption rate is larger than 5000 mol/s/m^3) are painted light gray.

concentration in the hot combustion gas stream downstream of the leading edge flame is very small. The thin oxygen diffusion layer is developed by molecular diffusion along the boundary between the hot combustion gas stream and the ambient atmosphere. It is found that the flame islands burn in this thin layer, and hence take the rather flat shapes as observed in Fig. 3. In the following, the ways in which the flame islands, high consumption rate volumes, come out locally and survive in the oxygen diffusion layer are discussed.

4.2. *Intensification and production of diffusion flame islands by inner rich premixed flame*

The combustion of diffusion flame islands decays, as time goes on and as they flow downstream because the hydrogen in the diffusion layer is

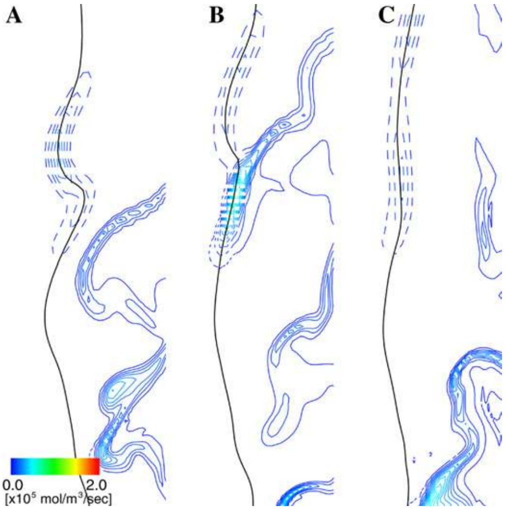

Fig. 5. The time evolution of hydrogen consumption rate distribution in a cutting plane. Premixed and diffisive consumption are drawn with solid and dashed lines, respectively, with an interval of 5000 mol/s/m^3. Stoichiometric mixture fraction lines are drawn with thick black lines. The time-stages correspond to those in Fig. 4.

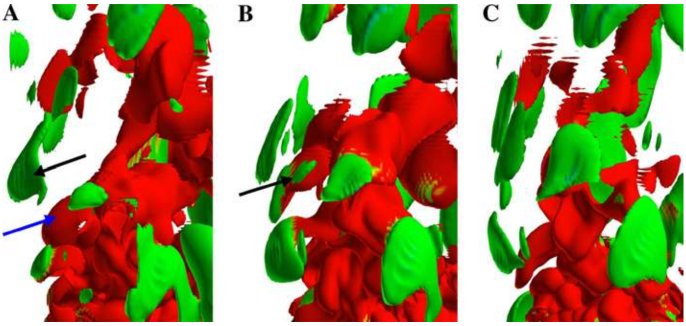

Fig. 4. Intensification process of a diffusion flame island by contact with the inner rich premixed flame. Iso-surfaces of hydrogen consumption rate at 10^4 mol/s/m^3 are drawn with a time interval of 47.6 μs. Surface color shows the combustion mode, red: rich premixed, blue: lean premixed, and green: diffusion.

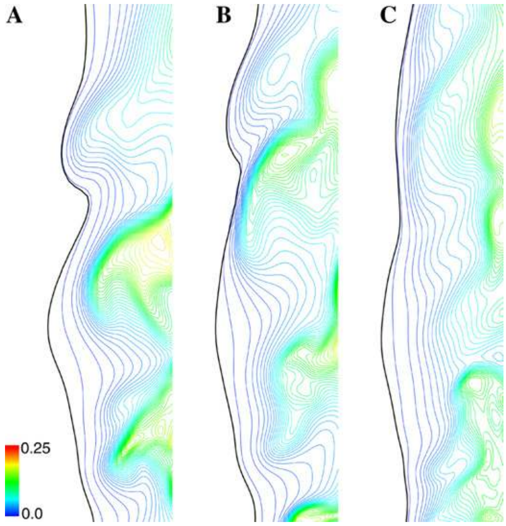

Fig. 6. The time evolution of hydrogen mass fraction distribution. The iso-lines are drawn from 0.005 to 0.25 with an interval of 0.005. Stoichiometric mixture fraction lines are drawn with thick black lines. The time-stages correspond to those in Fig. 4.

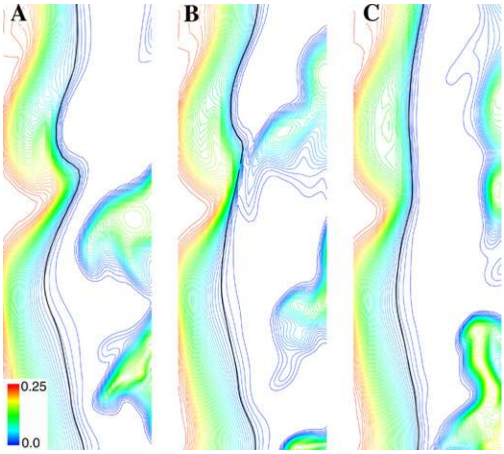

Fig. 7. The time evolution of oxygen fraction distribution. The iso-lines are drawn from 0.005 to 0.25 with an interval of 0.005. Stoichiometric mixture fraction lines are drawn with thick black lines. The time-stages correspond to those in Fig. 4.

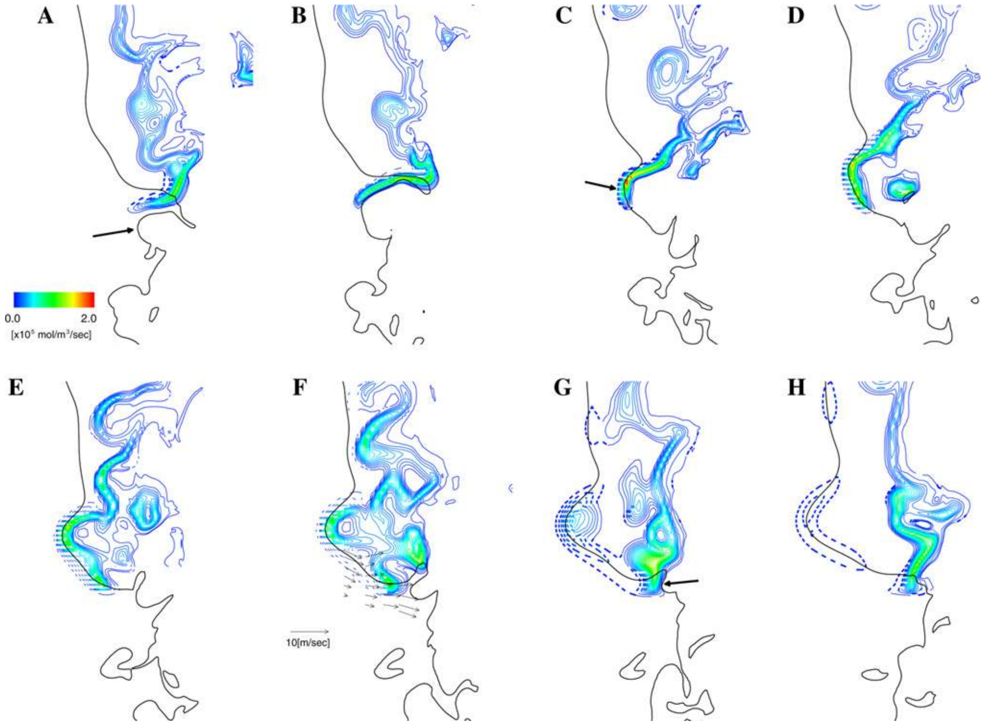

Fig. 8. Transformation of the leading edge flame structure and production of a diffusion flame island. The time evolution of hydrogen consumption rate distribution is presented with an interval of 5000 mol/s/m^3. Stoichiometric mixture fraction lines are drawn with thick black lines. The time interval is 0. 238 μs. The reference velocity vector corresponds to 10 m/s in (F).

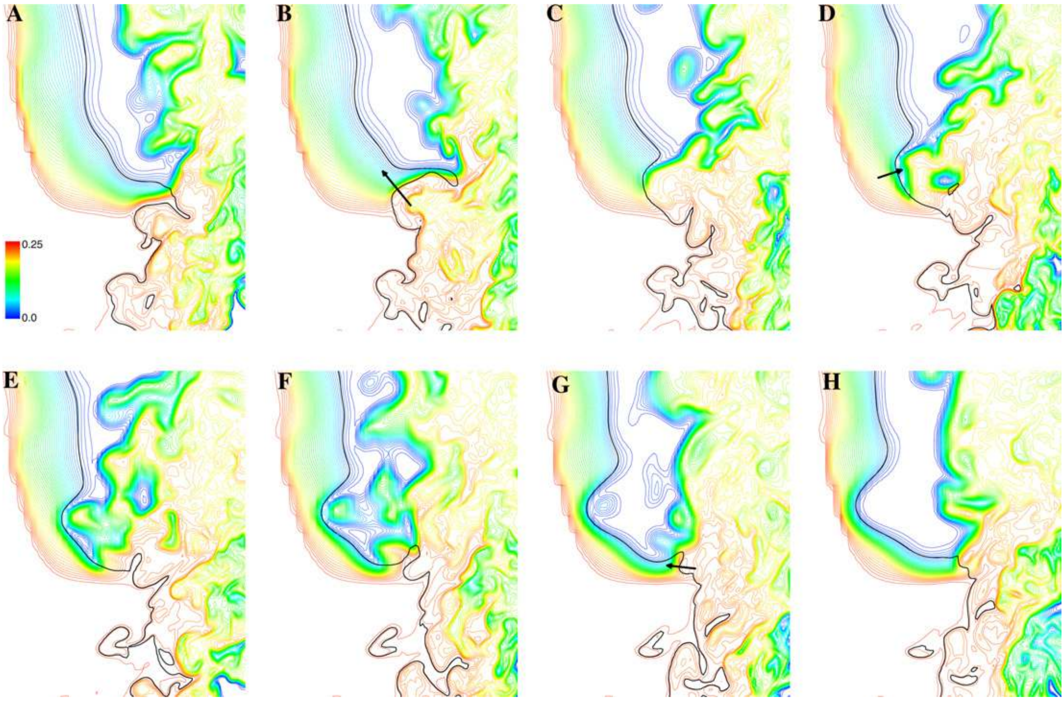

Fig. 9. The time evolution of oxygen mass fraction distribution during the transformation of the leading edge flame structure. The iso-lines are drawn from 0.005 to 0.25 with an interval of 0.005. Stoichiometric mixture fraction lines are drawn with thick black lines. The arrows in (B), (D), and (G) indicate the direction of the oxygen concentration gradient. The time-stages correspond to those in Fig. 8.

gradually consumed. But when a diffusion flame island comes into contact with the fluctuating inner rich premixed flame, the combustion is intensified.

Figures 4A–C show the three-dimensional views of an example process. The black arrow in Fig. 4A indicates the flame island of discussion. Figures 5–7 are the corresponding two-dimensional distributions of the hydrogen consumption rate, the hydrogen mass fraction, and the oxygen mass fraction, respectively. The window frame is from $[-2D, 8.5D]$ to $[0, 16D]$ where the coordinate origin is the center of the nozzle exit. The time interval between adjacent figures is 47.6 μs.

The inner rich premixed flame, which is vigorously unstable [1], sometimes locally comes into contact with a diffusion flame island when it moves outward largely. Part of the inner rich premixed flame, which is indicated by the blue arrow in Fig. 4A, comes across the flame island. Then, a transient flame configuration composed of diffusion and premixed flames, which are attached to each other, is formed, as indicated by the black arrow in Fig. 4B. The hydrogen in the rich mixture is conveyed to the oxygen diffusion layer, and the molecular diffusion of hydrogen to the reaction layer increases, as indicated by the high concentration of the iso-lines near the flame island in Fig. 6B. Then, the combustion in the flame island is intensified, as presented in Fig. 5B. The oxygen is also conveyed as observed in Fig. 7B, and the molecular diffusion of oxygen may decrease, but the effect is very small because the conveyed mixture is very rich and a large part of the oxygen has been consumed by the rich premixed flame.

The inner premixed flame moves downstream much faster than the diffusion flame island, and the oxygen in the connection layer is consumed. Then, the oxygen is exhausted as seen in Fig. 7C, leading to local extinction in the premixed flame, and the diffusive reacting volume is detached from the inner premixed flame to be a flame island again (Figs. 4C and 5C). The consumption rate in the diffusion flame island begins to decrease in accordance with the decrease of hydrogen concentration in the fuel side after the detachment.

So many wrinkles of the inner premixed flame pass by a diffusion flame island, and some of them encounter a contact with the flame island to intensify diffusive combustion. The discussed diffusion flame island experiences the above process several times during the observation.

The production of a diffusion flame island takes place by the same mechanism that is described above, although the details of the process are not mentioned here. When the inner rich premixed flame happens to come in contact with the oxygen diffusion layer, diffusive combustion is activated locally, leading to the production of a flame island in the oxygen diffusion layer.

5. Production of diffusion flame islands by leading edge flame unsteady behavior

The long-term observation reveals the production of diffusion flame islands by the unsteady behavior of the leading edge flame. When a relatively large unburned gas volume penetrates the leading edge flame, the leading edge transforms its structure. In the transformation process, a diffusion flame island comes out. Relatively small diffusion flame islands are observed near the base flame in Fig. 1. They are produced by this process.

The leading edge flame has a triple flame like structure when the flame motion is calm, and it is stabilized by the balance between the burning velocity and incoming gas velocity at the lean branch [1]. The stable structure disappears locally when a large unburned gas volume penetrates the leading edge flame. Figures 8A–H show an example process of the transformation of the leading edge flame structure in terms of the hydrogen consumption rate. The window frame is from [$-4D$, $4D$] to [0, $28/3D$]. The time interval is 23.8 μs. Figures 9A–H show the time evolution of the oxygen mass fraction distribution at the same time stages as in Figs. 8A–H.

In Fig. 8A, the leading edge flame is composed of lean/rich premixed branches and a weak diffusive branch. The large projection of the stoichiometric line, to which an arrow is pointed, indicates the approach of a rich unburned gas volume along the edge of the unburned hydrogen jet. The arrival of the rich unburnt gas volume shifts the lean branch toward the stoichiometric or rich condition (Fig. 8B), but diffusive reaction has not been produced by this event.

As the unburned volume penetrates the burned gas, the structure of the leading edge flame is transformed. The inner part of the leading edge flame is pushed downstream to make the reaction layer rather parallel to the axial direction, and the outer end of the reaction layer is pushed slightly outward (Figs. 8C and D). In this process, relatively strong diffusive combustion appears (see the green dashed iso-lines indicated by an arrow in Fig. 8C). As shown in Figs. 9C and D, a considerable amount of oxygen has been consumed in the reaction layer by premixed combustion, and thus the oxygen concentration gradient points from lean side to rich side across the flame, while it points from rich to lean when the lean branch exists (Figs. 9A and B). The arrows in Figs. 9B and D show the directions of the oxygen concentration gradient across the flames. Change in the concentration gradient results in a change in combustion mode.

As shown in Figs. 9E and F, the rich premixed flame, which is attached to the diffusion flame, goes toward extinction because the oxygen in the premixed flame is consumed. On the other hand, the diffusive mode maintains its combustion because oxygen is supplied by molecular diffusion from the ambient atmosphere. Then, after a while, the diffusion flame is detached from the rich premixed flame due to the local extinction of the rich premixed flame as shown in Fig. 8G. Figures 9F and H clearly illustrate the deficiency of oxygen in the extinction region.

The passage of the gas volume induces a flow inward and slightly upstream as shown in Fig. 8F, where the two-dimensional velocity vectors are drawn around the leading edge. The leading edge of the reaction layer moves on the induced flow. When the leading edge reaches the end of the projection of the stoichiometric line, the oxygen concentration gradient is from inside to outside, as is indicated by an arrow in Fig. 9G, while the hydrogen concentration gradient, which is nearly normal to the stoichiometric line for unburned gas, is from inside to outside. Then, the lean premixed combustion mode again appears as shown in Fig. 8G (see the solid iso-lines indicated by an arrow). During this period, the diffusive combustion becomes gradually weak due to the consumption of unburned hydrogen. The volume that contained a relatively large amount of hydrogen survives as a diffusion flame island at a distance from the leading edge of the flame and flows downstream slowly (Fig. 8H).

6. Conclusions

A hydrogen jet lifted flame was simulated by DNS approach over a significantly long period. From observation of the unsteady flame behavior, the following conclusions are obtained concerning the formation of the diffusion flame islands.

1. A thin oxygen diffusion layer is developed along the outer boundary of the lifted flame. Diffusion flame islands burn in the diffusion layer taking a rather thin shape.
2. Hydrogen consumption rate in a diffusion flame island is increased when it comes into contact with fluctuating inner rich premixed flame. Diffusive combustion is intensified by the unburned hydrogen supply from the fuel rich gas mixture to the oxygen diffusion layer. The production of diffusion flame islands also takes place by this procedure.
3. When a relatively large unburned gas volume penetrates the leading edge flame, the structure of the leading edge flame transforms. In the transformation process, a diffusion flame island

is produced. The local deficiency of oxygen is the key phenomenon for the appearance of diffusive mode combustion and for the formation of the island like structure.

In Fig. 1, the island like structure is observed not only in diffusion flames but also in the inner turbulent rich premixed flame. The production process of rich premixed flame islands will be investigated in the future work. The transformation of the leading edge flame structure seems to be very important for the stabilization of the leading edge flame, as well as for the production of diffusion island flames. This process should be investigated from the viewpoint of the flame stabilization mechanism.

The grid spacing increases gradually as the distance from the nozzle axis is larger than 1.25D. When the leading edge flame moves largely outward, high turbulence intensity and the thin premixed reaction layers may be conveyed outward leading to the lack of resolution. The same simulation with more than twice resolution in each space direction is being conducted using about 400 million grid points. As for the global structure of the flame, no significant difference has been observed, but the grid dependency on the detailed structure should be investigated.

Acknowledgment

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Comments

Forman A. Williams, UC-San Diego, USA. Your criteria for the existence of islands of diffusion flames must in some way be dependent on numerical tolerances. Your methods seem to identify diffusion flames when they are thin and strong, but where gradients of mixture fraction are much weaker you may not be able to detect the weak diffusion flames, which must be present unless they are extinguished by radiant energy loss.

Reply. As you point out, there is weak diffusive hydrogen consumption along the stoichiometric plane that we do not visualize. The diffusive consumption is very weak because the fuel side mixture is largely diluted with the products produced around the leading edge flame, but when the inner rich premixed flame conveys fresh hydrogen to the stoichiometric plane the diffusive consumption is amplified locally and the consumption rate becomes distinctively larger than in the neighbors. We call such amplified diffusive consumption volumes ‘diffusion flame islands’ in this study.

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Heinz Pitsch, Stanford University, USA. In your analysis you concentrate on the formation of rich islands by H_2 leaking through the rich premixed leading edge flame. However, since the stoichiometric surface is a closed surface surrounding the rich part of the flame, there always are reactive diffusive layers at the stoichiometric surface with fuel on one side and oxygen on the other. The reason why these appear like islands is that in some regions the scalar dissipation rate is higher than in others. It would therefore be more interesting to study why regions of high dissipation rate appear.

Reply. As you point out, there is a reactive-diffusive layer along the stoichiometric plane and the regions where the consumption rate is distinctively large appear like flame islands. When we look at the distribution of the scalar dissipation rate of the mixture fraction, the scalar dissipation rate is distinctively larger in the diffusion flame islands than in other locations. As far as we observed, the major increase of the scalar dissipation rate is caused by the approach of the rich gas mixture through the inner rich premixed flame or the rich branch of the leading edge flame.

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Norbert Peters, RWTH Aachen, Germany. Did you observe any leakage of hydrogen across the surface of stoichiometric mixture into the surrounding air?

Reply. We have not observed this phenomenon. The radial momentum of the inner turbulent hydrogen jet seems to have been dissipated when it reaches the stoichiometric plane through the dissipative burnt hot gas mixture.

●

Kai Luo, University of London, UK. From our experience, DNS of a 3-D lifted flame with complex chemistry at such a high Reynolds number would require many more grid points than the 23 million used. Using refined grids only in the reacting zones cannot solve the problem completely, because there are too many reaction zones. Can you explain how your simulation was stabilized numerically?

Reply. In our simulation, the grid is refined around the hydrogen jet core and the leading edge flame, and becomes coarser far downstream and at large radius. From the viewpoint of capturing the flow scales, it is not so critical because the flow scales become larger due to the high temperature inside the flame. But lack of resolution may occur from the viewpoint of resolving the reaction layers especially far downstream. Our scheme is spatially third-order in the smooth region, but falls into a fully upwind second-order scheme around weak extrema and even into a first-order scheme around very strong extrema. The strong numerical dissipation of first-order scheme may stabilize the simulation far downstream. To check the grid resolution effects, we have made two types of higher resolution simulation. In the first simulation, with 200 million grid points, we have simulated the same flame with the constant resolution that is as fine as the finest resolution in the present simulation. In the second, the resolution is twice but becomes coarse far downstream and at large radius and 400 million grid points are used. In both simulations, no significant differences have been observed with regard to the global flame structure. We believe the present simulation captures most of the essence of the flame.