Numerical Studies of Reacting Flows over Flat Walls with Fuel Injection*

(Part 2: Triple-Structure/Stabilization of a Diffusion Flame)

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A numerical study is performed on a two-dimensional, chemically reacting boundary layer to achieve a physical understanding of the stabilization and triple structure of a bulk flame. A theoretical model is presented to couple fluid dynamics, chemical kinetics and heat transfer at the surface of a flat wall. Computations are carried out at different Nusselt numbers and Reynolds numbers based on the free stream velocity. When the Nusselt number is increased, the flame apex begins to leave the wall surface and this manifests an unstable process. Finally it is blown off when the Nusselt number becomes sufficiently large. For a stable flame, three zones can be identified near the flame apex: a nonreactive mixing zone, a premixed/partially premixed flame zone and a diffusion flame zone. When the Reynolds number is decreased, the reaction zone develops away from the wall and more heat and fuel mass are transferred upstream of the burner, which is conducive to the stabilization of a bulk flame.

Key Words: Boundary Layers, Two-Dimensional, Laminar Flow, Combustion, Numerical Simulation

1. Introduction

In the past few decades, there has been increasing interest in the problem of structure and stability of diffusion flames within laminar boundary layers over a flat wall. This results, in part, from the fact that this problem is closely related not only to many practical applications such as combustion in hybrid rockets, fires over structures and liquid pools, but also to essential physical aspects of a system involving flow and combustion. Understanding and manipulating this problem require clear revelation of the fundamental interactions among the aerodynamics, chemical kinetics and heat transfer in reacting boundary layers over a flat wall.

One of the present authors investigated a diffusion flame established in laminar boundary layers over a flat wall with a chemical reaction without heat release⁽¹⁾, and used a flame sheet model to account for

a chemical reaction with heat release⁽²⁾. In these works were described the flow acceleration that induced an anomaly in velocity distribution, and the hydrodynamic instability that may disturb and wrinkle the flame sheet downstream. However, as fast chemistry was allowed, it was impossible to predict phenomena such as extinction and triple structure of a bulk flame, which have been observed frequently in related experiments. Sharing facets of the present work, some experimental and numerical studies have been carried out as well. Using a boundary layer theory, Emmons⁽³⁾ obtained profiles of concentrations, velocity and temperature within a boundary layer over a flat wall of solid fuel. According to that theory, however, the burning rate would become infinite at the leading edge of the condensed fuel wall. To describe the transition of a bulk flame, Hirano and co-worker^{(4),(5)} investigated experimentally the flame stabilizing mechanism by changing the velocity of injected gaseous fuel and the free stream. However, no details were reported on thermal and reaction zone structures when the bulk flame underwent a transition. Miyashita et al.⁽⁶⁾ conducted an experimental study of the effects of the free stream velocity on

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flame stabilization and found that, at a low velocity, a recirculation flow formed upstream of the burner could act as a stabilizer of the bulk flame. Using finite-rate Arrhenius kinetics, Chen and T'ien⁽⁷⁾ investigated the transition from an envelope to an open-tip flame when the Damköhler number decreases. However, equal molecular weight of reactants and temperature-independent diffusion coefficients were assumed with a constant wall temperature of the burner. To include the interaction between fluid mechanics and combustion, Kodama and Fernandez-Pello⁽⁸⁾ treated a diffusion flame stabilized over a solid fuel plate and studied the flame apex positions as a function of flow velocity. Combustion near the leading edge of the plate is precluded due to the use of an inert plate. In the present study, we are particularly concerned about an air stream flowing parallel over a flat wall. From a part of the surface of the wall (known as the burner), gaseous fuel is vertically injected into the air stream, mixed and reacted chemically with the oxidant. Under certain conditions, a bulk flame may be established and stabilized near the leading edge of the burner, so chemical reaction takes place and interacts closely with flow and thermal states, for instance, the rate of heat transfer at the wall surface and the velocity of the free stream, which may be represented by the Nusselt number and the Reynolds number.

2. Physical Model and Governing Equations

The computational domain shown in Fig. 1 is 350 mm long and 100 mm wide. Gaseous fuel is injected from part surface of the wall within a region from $x=40$ mm to 110 mm with uniform velocity, forming a burner 70 mm long. Chemical reaction occurs within the boundary layer and a bulk flame is formed and developed by allowing a main air stream containing both oxygen and nitrogen to flow over the horizontal flat wall. The governing partial differential equations of mass, momentum, energy and chemical species are deduced for two-dimensional laminar reacting flows. In a mathematical treatment of combustion, the chemical reaction model is a one-step, irreversible model with second-order, finite rate Arrhenius kinetics, and

can be expressed as:

The heat of chemical reaction is taken into account in this model, which has been widely used with much success in combustion problems in the zero Mach number limit and appears to cover the essential physics of many combustion phenomena. Details on other assumptions used in present study are given in Ref. (2). Although the use of a one-step overall reaction is inadequate for predicting details of chemical reactions and some related features, it is sufficient to predict the behavior of the overall structure of the flame and its interaction with a flowfield because of the reaction heat release. For the problem under question, as a significant temperature change occurs due to reaction heat release, it is important to deal with the temperature-dependent diffusion coefficients. Based on the assumptions, behaviors of the chemical reaction and its coupling with fluid dynamics can be obtained by solving conservation equations of the energy and the respective chemical species. The height of the computational domain is chosen as the characteristic length, and the state of the main air stream at $T_\infty=300$ K and at atmospheric pressure is specified as reference to normalize the governing equations. The dimensionless equations are as follows:

Continuity equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0, \quad (2)$$

Momentum equations

$$\begin{aligned} \frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho uu)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} \\ = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[\frac{\mu}{Re} \left(2\frac{\partial u}{\partial x} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right) \right] \\ + \frac{\partial}{\partial y} \left[\frac{\mu}{Re} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right], \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho vu)}{\partial x} + \frac{\partial(\rho vv)}{\partial y} \\ = -\frac{\partial p}{\partial y} + \frac{G_r}{Re^2} \frac{T-1.0}{T_f-1.0} \\ + \frac{\partial}{\partial x} \left[\frac{\mu}{Re} \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] \\ + \frac{\partial}{\partial y} \left[\frac{\mu}{Re} \left(2\frac{\partial v}{\partial y} - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right) \right], \end{aligned} \quad (4)$$

Fig. 1 Physical model for the computation

Energy equation

$$\frac{\partial(\rho T)}{\partial t} + \frac{\partial(\rho u T)}{\partial x} + \frac{\partial(\rho v T)}{\partial y} = \frac{\partial}{\partial x} \left(\frac{\mu}{Re Pr} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\mu}{Re Pr} \frac{\partial T}{\partial y} \right) + Q \omega_{fu}, \quad (5)$$

Chemical species

$$\frac{\partial(\rho Y_i)}{\partial t} + \frac{\partial(\rho Y_i u)}{\partial x} + \frac{\partial(\rho Y_i v)}{\partial y} = \frac{\partial}{\partial x} \left(\frac{\mu}{Re Sc} \frac{\partial Y_i}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\mu}{Re Sc} \frac{\partial Y_i}{\partial y} \right) + \omega_i, \quad (6)$$

$$T = T^*/T_\infty^*, Q = Q^*/C_p T_\infty^*, \mu = \frac{\mu^*}{\mu_\infty^*},$$

$$Pr = \frac{C_p \mu_\infty^*}{\lambda_\infty^*}, Sc = \frac{\mu_\infty^*}{\rho_\infty^* D_\infty^*}, \quad (7)$$

where ρ, u, v, p, T, Y_i are the density, velocity components of the x - and y -directions, pressure, temperature and mass fraction of i th chemical species for the mixture gas, respectively. The superscript * indicates dimensional quantities and the subscript ∞ , free stream quantities. The consumption rate of the fuel is

$$\omega_{fu} = -Da \rho^2 Y_{fu} Y_{ox} \exp(-Z/T), \quad (8)$$

where Da is the Damköhler number and Z , the Zel'dovich number, defined as follows:

$$Da = B_f H \rho_\infty^* / U_\infty^* W_{ox}, Z = E/RT_\infty^*,$$

B_f is the pre-exponential coefficient and W_{ox} is the molecular weight of the oxidant. Four species of fuel, oxidizer, inert and product are taken into account. The equation of the thermodynamic state is

$$\rho = \frac{p}{C_1 T}, \quad (9)$$

where $C_1 \equiv RT_\infty^* / U_\infty^* = 1/kM^2$, k is the specific heat ratio of the gas mixture, M is the Mach number of free stream flow and R is the gas constant of the mixture estimated by

$$R = \sum_{i=1}^n \frac{Y_i}{W_i} R_u. \quad (10)$$

In Eq. (10), R_u is the universal gas constant and W_i is the molecular weight for i th species.

Boundary Conditions

At the inlet,

$$u = u(y), v = v(y), p = p^*/\rho_\infty^* U_\infty^* / U_\infty^*, \\ T = 1, Y_{fu} = 0, Y_{ox} = 0.233, Y_{n_2} = 0.767.$$

At the outlet,

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = \frac{\partial p}{\partial x} = 0, \\ \frac{\partial T}{\partial x} = \frac{\partial Y_{fu}}{\partial x} = \frac{\partial Y_{ox}}{\partial x} = \frac{\partial Y_{n_2}}{\partial x} = 0.$$

At the upper boundary,

$$\frac{\partial u}{\partial y} = \frac{\partial v}{\partial y} = \frac{\partial p}{\partial y} = 0, \\ \frac{\partial T}{\partial y} = \frac{\partial Y_{fu}}{\partial y} = \frac{\partial Y_{ox}}{\partial y} = \frac{\partial Y_{n_2}}{\partial y} = 0.$$

At the lower boundary,

not on the burner surface,

$$\frac{\partial Y_{fu}}{\partial y} = \frac{\partial Y_{ox}}{\partial y} = \frac{\partial Y_{n_2}}{\partial y} = 0,$$

$$u = v = 0, -\lambda \frac{\partial T}{\partial y} = h(T - 1);$$

on the burner surface,

$$\frac{\partial Y_{fu}}{\partial y} = \dot{m} + \frac{1}{Re Sc} \mu \frac{\partial Y_{fu}}{\partial y},$$

$$\frac{\partial Y_{ox}}{\partial y} = \frac{1}{Re Sc} \mu \frac{\partial Y_{ox}}{\partial y},$$

$$\frac{\partial Y_{n_2}}{\partial y} = \frac{1}{Re Sc} \mu \frac{\partial Y_{n_2}}{\partial y},$$

$$u = 0, v = v_w, -\lambda \frac{\partial T}{\partial y} = h(T - 1),$$

Referring to Lee and T'ien's work⁽¹⁰⁾ on the gas-phase chemical reaction where the fuel is taken as methane (CH_4), the values of related properties are specified: $Pr = 0.714$ and $Q^* = 116.8$. Injection velocity of the fuel v_w is chosen as 7 cm/s, which corresponds to the experimental conditions⁽¹¹⁾ in which a stable bulk flame may be steadily established. The governing equations are numerically integrated by SIMPLE procedure and many numerical experiments have been done to properly specify the size of the computational domain and the mesh. A nonuniform mesh is adopted with grid nodes 400×145 .

3. Results and Discussion

Many computations are performed and five typical cases are chosen to focus at the effects of the Nusselt number and the Reynolds number based on the free stream velocity. By varying these parameters, bulk flames undergoing a transient process have been simulated numerically. Parameters of the five cases are listed in Table 1.

Injecting velocity of the fuel is fixed at 0.07 m/s in all the five cases and the free stream velocity is set at 1 m/s in the first three cases. The effects of varying free stream velocity are reflected in cases 4 and 5. The determination of these velocities is based on the

Table 1 Computed cases

Case No.	Re	$Nu_{(\delta y)}$	Da
Case 1	6234	0.05	1.85×10^8
Case 2	6234	0.062	1.85×10^8
Case 3	6234	0.07	1.85×10^8
Case 4	3117	$0.05\sqrt{0.5}$	$\frac{1.85 \times 10^8}{\sqrt{0.5}}$
Case 5	8104	$0.05\sqrt{1.3}$	$\frac{1.85 \times 10^8}{\sqrt{1.3}}$

experimental study in which stabilized and transient bulk flames have been observed⁽¹¹⁾.

3.1 Varying Nusselt number

The Nusselt number is defined as $h \Delta y / \lambda$, where h is the heat transfer coefficient, λ , the heat conductive coefficient and Δy , an interval between the first node and the wall. As the Nusselt number is proportional to the heat transfer coefficient, its increase will result in an increase in heat transfer from the gas phase to the solid flat wall at fixed values of Δy and λ . The effect of varying the Nusselt number is investigated by fixing the free stream velocity and by changing h over a wide range in cases 1, 2 and 3. Contours of nondimensional reaction rate of the fuel are depicted in Fig. 2 for the three cases. One common fact that can be noticed is the chemical reaction concentrating in the apex of the reaction zone, meaning that a highly exothermic zone exists there and serves as a holder to stabilize the bulk flame. At $Nu=0.04$ in Fig. 2 (a), the reaction zone anchors at the surface of the wall and originates from upstream of the leading edge of the burner at $x=0.4$, forming an enveloped flame and preheating the cold oxidizing stream before penetrating into the fuel side. This implies that the fuel is carried, mixed and reacted chemically upstream of the burner and some quantitative results will be shown later. When the Nusselt number is increased as in cases 2 and 3, the chemical reaction zones are shrunk downstream and their apexes become open and no longer anchor at the surface of the flat wall. This indicates the generation of a low-temperature zone between the flame apexes and the surface of the wall, where only the mixing of the fuel and oxidizer takes place until the temperature is high enough to bring about and sustain the chemical reaction. This phenomenon has been observed in many experiments that at certain conditions, there exists a premixed zone of the fuel and the oxidizer near the apex of the bulk flame. Also, it can be seen that increasing the Nusselt number increases the chink of the open tip, leading to enforce deformation and downstream shrinkage of the apex of the reaction zone because heat loss increases through the wall and temperature decreases at the surface of the wall. Contours of the nondimensional temperature are shown in Fig. 3 for the three cases. For case 1 at $Nu=0.04$, contours of the high-temperature zones are enclosed upstream of the leading edge of the burner and high streamwise gradients appear there; thus, a large heat flux moves upstream to preheat the cold oxidizing stream. When the Nusselt number is increased as in cases 2 and 3, however, the high-temperature zones are lifted off and blown downstream, resulting in less heat transfer upstream and lower temperature zones near the

Fig. 2 Contours of reaction rate of the fuel for three Nusselt numbers. (a) case 1, (b) case 2 and (c) case 3

Fig. 3 Contours of the temperature for three Nusselt numbers. (a) case 1, (b) case 2 and (c) case 3

apexes of these contours. Thus, chemical reaction is hard to sustain there, as shown in Fig. 2, and stabilization of the flames is weakened. A further decrease in the Nusselt number will bring about a situation in which the flame may be blown off downstream and stabilize near the rear edge of the burner, or disappear from the computational zone. This explains the transient processes of the bulk flame from an enveloped one to an open-tip one due to the change in the heat loss through the surface of the wall.

To clarify the stability and the transition of a bulk

Fig. 4 Profiles of the mass fractions of the fuel and the oxidant for six streamwise positions over the burner. (a) case 1, (b) case 2 and (c) case 3

flame near the leading edge of the burner, it is important to know the details of the diffusion process of the chemical species arising there. Figure 4 gives profiles of mass fractions of the oxidizer and fuel along the y -direction at six streamwise positions near the leading edge of the burner at $x=0.4$ for cases 1, 2 and 3. Curves of the oxidizer profiles are indicated by dashed lines and curves of the fuel, by solid ones. In case 1, because an enveloped flame is stabilized upstream of the leading edge of the burner, mass fractions of the fuel and the oxidizer reach zero almost at the same spatial position, indicating the establishment of a diffusion-controlled flame. At positions $x<0.6$ in cases 2 and 3, a zone at which both oxidizer and fuel

coexist, that is, a premixed zone of the two reactants, is clearly recognized, which is located adjacent to the wall and tends to extend vertically downstream of the leading edge of the burner. Considering that the streamwise location of the apex of the reaction zone is at $x_{apex2}=0.4635$ in case 2 and at $x_{apex3}=0.5607$ in case 3 as shown in Fig. 2, three stages can be recognized along the x -direction. First of all, the fuel and the oxidizer are mixed by diffusion and convection and chemical reaction does not take place until x_{apex2} and x_{apex3} , thus, a premixed zone of the reactants is formed. Downstream of the x_{apex2} and x_{apex3} , a chemical reaction is initiated and the generation of premixed/partially premixed flames is expected. It is also noted that the stoichiometry of the premixed flame varies from fuel rich near the wall, to fuel lean far away the wall along the y -direction. Premixed zones, however, remain at least till $x=0.4675$ in case 2 and $x=0.6075$ in case 3 as the mixed reactants have not been consumed completely due to the low temperature, and consequently the low reaction rate. At $x=0.7075$, a diffusion flame is achieved since the mass fractions of both the fuel and the oxidizer approach zero at a same spatial position. This is known as a triple flame structure that has been discussed in other researches^{(12),(13)}. It is reasonable to infer that there exist transient flames from a premixed one, through a comparably predominant one by both chemical kinetics and diffusion, and to a diffusion one. When the Nusselt number is increased, profile gradient of the fuel adjacent to the wall decreases, especially near the leading edge of the burner at $x=0.4$. This tendency diminishes downstream. The diffusion height (the vertical distance from the wall to a position where mass fraction of the fuel reaches zero) is smaller in case 1 than in cases 2 and 3, but no obvious distinction appears between the latter two cases.

Profiles of the temperature at the six streamwise positions are shown in Fig. 5 for the three cases. A common change in the profiles is found, i.e., when y is increased, the temperature increases mildly in the fuel side (refers to an area below the reaction zone in this paper), peaks at the reaction zone, and decreases sharply in the oxidizer side (above the reaction zone). In case 1, for the low Nusselt number, a maximum temperature above 6.0 is achieved at $x=0.3975$ and value of the maximum temperature tends to decrease downstream. When the Nusselt number is increased as in cases 2 and 3, the temperature is very low near $x=0.4$ so there is no chemical reaction that takes place, as shown in Fig. 2; the high-temperature zone can only be found in the rear part of the burner.

To obtain an insight into the heat transfer between the free stream and the wall, it is necessary to

Fig. 5 Profiles of the temperature for six streamwise positions over the burner.
(a) case 1, (b) case 2 and (c) case 3

Fig. 6 Profiles of the temperature (a) and its gradient
(b) for the three cases

understand the thermal features of the wall surface. The distributions of the temperature and its y -direction gradient on the wall surface are shown in Figs. 6 (a) and 6(b) respectively. Some similarity can be seen in the two figures, i.e., the profiles increase very rapidly, peak close to the apexes of the bulk flames, then fall with further increase in x . This trend of temperature change is consistent with many experimental results. When the Nusselt number is increased, the maximum temperature on the wall surface decreases and the corresponding position moves downstream.

The variation of the Nusselt number may affect the aerodynamic structures of the boundary layer. Therefore, its effect is examined using contours of the streamwise velocity component depicted in Fig. 7. The profiles of the velocity at six streamwise positions are also shown in Fig. 8. In Fig. 7, the bold contour lines mean negative values, and a recircula-

tion flow zone and a stagnation point are clearly observed near the leading part of the burner. The recirculation zone enlarges and the stagnation point is transferred downstream with increasing the Nusselt number. In particular, the recirculation zone is formed and covers a part of the surface of the burner. Because of the recirculation zone, the fuel mass is transferred upstream. Therefore, the premixed zone of the fuel and the oxidizer is observed and enlarged upstream of the burner. This has been identified by the nonzero fuel mass fraction at $x=0.3975$ as shown in Fig. 5. Small recirculation zones are observed near $x=0.8$, which are leading parts of the recirculation zones located downstream of the rear edge of the burner at $x=1.1$ where fuel injection ends. In Fig. 8, the velocity profiles near $x=0.4$ are quite different, that is, up to $y=0.05$, the velocity approaches a local positive maximum due to the presence of an enveloped bulk flame there in case 1, while it

approaches a local negative maximum due to recirculation zones in cases 2 and 3. Further downstream, the velocity reaches a maximum value exceeding the free stream velocity, which is known as the "velocity overshoot" phenomenon and is reproduced by the numerical simulation.

Contours of vorticity are shown in Fig. 9 for the three cases, in which positive and negative values of the vorticity are indicated by thin and bold lines, respectively. In all three cases, a large zone of positive vorticity is clearly observed to overlap with the chemical reaction zone, as well as a small one within the recirculation zone. The large zone is surrounded by a zone at which negative vorticity is predominant. The formation of the zone is responsible for the thermal expansion and for the effect of baroclinic torque,

Fig. 7 Contours of the streamwise velocity component for three Nusselt numbers. (a) case 1, (b) case 2 and (c) case 3

Fig. 8 Profiles of the streamwise velocity for six streamwise positions over the burner. (a) case 1, (b) case 2 and (c) case 3

as described in Ref. (2). Behaving as the reaction zone, the leading part of the zone moves downstream and is lifted away from the wall with increasing the Nusselt number. The formation of the small zone is definitely attributed to the recirculating flow there. The size of the small zone tends to increase with increasing the Nusselt number in both the x - and y -directions. Since positive vorticity is closely related to thermal expansion, the patterns of vorticity contours are affected severely by the temperature field (see Fig. 3). Counter-rotation vortices may potentially develop downstream and may cause disturbances of the flowfield and the flame.

3.2 Varying Reynolds number

To examine the effect of the Reynolds number based on the free stream velocity, The results of cases 1, 4 and 5 are chosen at three velocities, i.e., $u=1$ m/s, 0.5 m/s and 1.3 m/s. The results of case 1 are used as the common case in this section so that the extent of the influence of the Reynolds number may be easily discerned. Most of the results of case 1 have been given in section 3.1 even if the following discussion covers the three cases. Only the results of cases 4 and 5 will be given here.

The contours of the nondimensional reaction rate of the fuel are depicted in Fig. 10 for cases 4 and 5. On comparison with Fig. 2(a), it is found that the chemical reaction takes place upstream of the burner in all three cases. However, the apex of the reaction zone anchors at the surface of the wall in cases 1 and 4, while a chink appears in case 5 because of comparatively more heat loss through the wall surface and less time for reactants to mix. When the Reynolds number is decreased, the boundary layer becomes thicker and it is possible for the fuel to diffuse farther from the wall, so the rear part of the reaction zone is lifted and moves farther away from the wall. According to the

Fig. 9 Contours of the vorticity for three Nusselt Numbers. (a) case 1, (b) case 2 and (c) case 3

Fig. 10 Contours of reaction rate of the fuel for two Reynolds numbers. (a) case 4 and (b) case 5

values in the parentheses, the maximum value of the reaction rate does not vary markedly between cases 1 and 4, but decreases rapidly when the velocity increases to 1.3 m/s in case 5. Above 1.3 m/s, the bulk flame becomes very unstable and sensitive to the velocity. A further increase in the velocity results in blowing off or extinction of the bulk flame. Contours of the temperature are shown in Fig. 11 for cases 4 and 5. The thickness of the thermal boundary layer becomes smaller and the temperature change becomes more marked towards the air side with increasing the Reynolds number. This result is qualitatively consistent with many experimental observations and measurements.

Profiles of the oxidizer and fuel mass fractions are given in Fig. 12 at six streamwise positions around the leading edge of the burner ($x=0.4$) for cases 4 and 5. Premixed zones of the reactants can hardly be found

Fig. 11 Contours of the temperature for two Reynolds numbers. (a) case 4 and (b) case 5

Fig. 12 Profiles of the mass fractions of the fuel and the oxidant for six streamwise positions. (a) case 4 and (b) case 5

in the two cases, which is consistent with the distribution of the reaction zones shown in Fig. 10; intersecting points of the profiles of the two reactants move farther away from the wall in case 4 than in case 5, meaning that the flame height increases with decreasing the velocity. Profiles of the temperature at the six streamwise positions are shown in Fig. 13 for cases 4 and 5. The trends common to the profiles are as follows: the maximum temperature appears to

Fig. 13 Profiles of the temperature for six streamwise positions over the burner. (a) case 4 and (b) case 5

Fig. 14 Profiles of the temperature (a) and its gradient (b) for three different Reynolds numbers

change less along the x -direction, and the temperature at the wall surface ($y/L = 0$) decreases monotonically downstream in the two cases. The reason for the latter is that the heat transfer from the reaction zone to the wall decreases because the reaction zone moves away from the wall downstream. Also it is found that when the velocity decreases, the temperature gradient in the fuel side becomes small because of the thick thermal boundary layer. Corresponding distributions of the wall temperature and its gradient are shown in Fig. 14 along the x -direction. Values of the wall temperature and its gradient are largest in case 1 and smallest in case 4. The temperature increases at the most upstream position in case 5, and at a slightly downstream position in cases 1 and 4. This implies that among the three cases, heat is transferred most upstream in case 5 because of its highest streamwise temperature gradient. Other reasons related to this is further discussed together with

Fig. 15 Contours of the streamwise velocity component for two Reynolds numbers. (a) case 4 and (b) case 5

aerodynamic structures of the boundary layers in the following. Contours of streamwise velocity and their profiles at six positions are depicted in Figs. 15 and 16,

Fig. 16 Profiles of the streamwise velocity component for six streamwise Positions. (a) case 4 and (b) case 5

Fig. 17 Contours of the vorticity for two Reynolds numbers. (a) case 4 and (b) case 5

respectively, for cases 4 and 5. Values of the two extremes of the contours are shown in the parentheses. Together with Fig. 7(a), it can be seen that there exists a largest and strongest recirculation zone with the largest negative streamwise velocity, but the smallest velocity overshoot in case 5. The recirculation has contributed significantly to the heat transfer upstream from the apex of the flame. According to Figs. 16 and Fig. 8(a), the velocity overshoot is very obvious and the position of the peak velocity is very far from the wall due to the extremely thick boundary layer in case 4. Contours of vorticity are shown in Fig. 17 for cases 4 and 5. By comparing with Fig. 9(a), it can be seen that, among the three cases, the zone of positive vorticity along the reaction zone is the broadest and the value of maximum positive vorticity is the largest in case 4. This can be explained using Fig. 16: after the velocity peaks at $y \approx 0.1$, it decreases with increasing y and approaches the free stream velocity, meaning that $\partial u / \partial y$ is less than zero and that the formation of a positive vorticity

zone is possible according to the definition of vorticity; the range of y where $\partial u / \partial y < 0$ is the widest, so it results in the widest zone of positive vorticity among the three cases.

4. Conclusions

(1) A computational model is presented to couple fluid dynamics, chemistry and heat transfer at the surface of a flat wall. Computations are performed to obtain a physical understanding of the triple structure of the flame apex, the aerodynamic structure and the flame stability, by varying the Nusselt number and free stream Reynolds number.

(2) When the Nusselt number is increased, a bulk flame may manifest transient of enveloped, open-tip and blowing off processes. Meanwhile, from the profiles of the mass fractions of the reactants when a bulk flame is in an enveloped or an open-tip state, a triple flame structure and three zones can be identified in the streamwise direction, i.e., a nonreactive mixing zone, a premixed/partially premixed flame zone and a diffusion flame zone, which is consistent with some experimental observations.

(3) When the free stream velocity is decreased, the chemical reaction zone develops farther away from the wall and much more heat and fuel mass are transferred upstream of the burner, which aid to stabilize the apex of the flame. For a stabilized flame, the temperature and its gradient on the wall surface is maximal near the leading edge of the burner, then decrease rapidly downstream.

(4) In all cases, a recirculation flow can be observed upstream of the leading edge of the burner, which is responsible for the heat convection and movement of the flame apex upstream; a zone of positive vorticity is observed along the chemical reaction zone, and is

surrounded by a zone of predominantly negative vorticity. This indicates the presence of many counter-rotating vortices and a potentially disturbing source due to the motion and development of these vortices.

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