A Numerical Study on the Detailed Structure of Hydrogen/Air Bunsen Flame

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Abstract: The detailed flow, temperature and concentration fields of a hydrogen-air Bunsen flame have been examined by a precise numerical study that uses the exact transport properties and the full chemical reaction mechanism. The study has revealed that the chemical reactions along the flame cone portion do not remain uniform; the $H_2$ consumption rate decreases towards downstream. The decrease of $H_2$ concentration of the mixture coming into the cone, caused by the radial outward diffusion of mobile $H_2$ molecules, leads to the slowdown of the main $H_2$ consuming elementary reactions downstream. Circumferential curvature of the axisymmetric flame and thermal diffusion are not important in the observed behavior. It is also revealed that the structure of the flame tip is fundamentally two-dimensional, in the sense that the mixture coming into the tip continues the combustion reaction with a strong aid of heat diffusion from the outer flame cone. The result raises a serious question if the tip can be called a part of the self-sustained premixed flame.

Key Words: Bunsen flame, Flame structure, Flame tip, Flame cone, Flame curvature, Thermal diffusion

1. Introduction

The Bunsen flame is the most familiar laminar premixed flame and the cone-shaped flame is stabilized on the burner rim against the incoming mixture flow which is much faster than the normal burning velocity. The flame is stable in the upstream cone portion since the component of incoming velocity normal to the flame balances with the burning velocity [1-5]. However, at the flame tip on the central axis, the incoming flow is normal to the flame and is much faster than the burning velocity, and the mechanism by which the flame is stabilized at the tip has long been a controversial problem. In certain cases the tip is locally extinguished to cause the tip opening [1], and extensive experimental studies have been carried out by C.K. Law et al. to understand the physics associated with the variation in burning characteristics of Bunsen flames [6-10]. They proposed an idea to explain the observed tip behavior in terms of the burning velocity modification by the so-called preferential diffusion mechanism. This plausible explanation has attracted attention of the theoreticians and has accelerated studies to develop theories to predict the effects of Lewis number, stretch and curvature on the burning velocity [11-14]. These theories are basically extensions of one-dimensional flame theory and have been developed to understand turbulent flame behavior in terms of the laminar flamelet model [5]. On the other hand, no experimental observations that directly substantiate this preferential diffusion mechanism have been made so far because observing the details of 3D flow field and temperature and concentration fields in the narrow tip region is very difficult. At present, we still do not know accurately what is going on at the flame tip region, and before anything else, we have to understand the detailed tip structure. In addition, there are some experimental observations that the upstream flame cone portion does not always remain uniform, but the flame temperature decreases towards downstream [8]. Furthermore, a numerical study has shown that the maximum heat release rate along the cone decreases towards downstream. This happens for the lean hydrogen-air mixture, but is not clear for the stoichiometric mixture. It should be interesting to understand the reason how this non-uniformity is produced. Law et al. have explained this flame temperature behavior on the basis of preferential diffusion and stretch induced by flame curvature and insisted that the experimental observation correlates well with the theoretical prediction [8]. However, there have been no direct experimental observations that substantiate this explanation, here again.

Since experimental studies are very difficult, alternative ways of elucidating the flame structure should be sought and one possibility is numerical experiments. Recent progress in the field of numerical simulation has been remarkable [15], and we can make use of numerical calculation using exact transport
properties and full kinetics to reproduce what is going at the flame. One pioneering attempt has tried to understand flame tip behavior in terms of a global one-step reaction [13]. However, in the preferential diffusion problem, the individual behaviors of the chemical species involved in the reactions will have a major influence and so the simple global reaction model cannot correctly predict the tip behavior. A rather comprehensive numerical experiment with variable transport properties and a detailed chemical kinetics mechanism has been carried out to understand the effect of Lewis number, equivalence ratio, and velocity profile on the structure of a 2D H2/air Bunsen flame [12], but regrettably, overlooked the peculiar role played by the mobile H2 molecule. In addition, they have not yet made clear how the tip can be stabilized for the incoming fast flow. Ern et al. studied the effects of thermal diffusion on the hydrogen-air Bunsen flame, in a rather comprehensive numerical study with full kinetics and a detailed transport model [14], and concluded that the effect of thermal diffusion is significant.

We have started a program to understand the structure and behavior of the Bunsen flame by precise numerical experiment. In this first report we concentrate on the detailed structure itself. The tip opening mechanism will be studied in succeeding papers. In the following we describe the results of flame cone portion separately from those of flame tip. This is because we have found that the flame tip structure is completely different from that of 1D premixed flame.

2. Numerical Model

A hydrogen/air mixture is used, since the chemical reaction mechanism is relatively well-known and the numbers of elementary reactions; and chemical species involved are rather small. Figure 1 shows the numerical model adopted in this study. A hydrogen-air mixture of equivalence ratio 1 flows upwards with a parabolic velocity profile through a burner tube of 5.0 mm inside diameter and 45.0 mm height, and an axisymmetric flame cone is established on the burner tube. The ambient pressure is atmospheric. The velocity selected is 8 times the normal burning velocity of 1D flame at the center of the burner tube exit. We are mostly concerned with the flame tip on the axis, and hence the boundary conditions at the burner rim are kept as simple as possible. The tube wall is non-slip and adiabatic, except for the inner surface on which the temperature is kept below 400K to prevent the flame flash back. Hot burned gas of the same mixture fills the periphery of the tube to prevent an outer diffusive reaction with the atmosphere, and hence the flame can easily be stabilized at the rim of the tube.

The nine-species (H2, O2, OH, H2O, H, O, H2O2, HO2, N2) and 21-reaction model by Saxena and Williams [16] is employed for hydrogen/air reaction system. Table 1 shows the adopted reaction mechanism. The enthalpy and transport coefficients of each species are taken from CHEMKIN library [17]. The molecular diffusion coefficients in the mixture are estimated by mixture-averaged formulae, and the thermal diffusion effect is included for H2 and H. The air is assumed to be composed of 21% O2 and 79% N2 by volume. The governing equations are discretized by a

![Fig. 1 Numerical Model.](image-url)
finite volume method. The convective fluxes are evaluated using the 5th-order numerical flux constructed by characteristics-based WENO procedure [18] based on Roe’s scheme [19], and the diffusion fluxes by the 2nd-order central differential formulae. The simulation is conducted in an axisymmetric formulation except for the singular central axis. Finite computational volumes are allocated along the singular axis, and the conservation equations are solved separately. The tube inlet boundary conditions are given by the NSCBC method [20] imposing inlet velocity, temperature and gas mixture composition. At the outer boundaries, the non-reflection condition [20] is imposed for the outgoing flow and the total pressure and the total temperature are fixed for the incoming flow. The computational domain is [-9D, 17D] (axial)×[0,13D] (radial), where D is the tube inner diameter. The grid spacing is 12.5μm around the flame and a finer grid is adopted near the wall boundaries. A corresponding 1D normal flame structure, to be compared with the 2D axisymmetric flame structure, is calculated by using CHEMKIN PREMIX Code [17].

3. Numerical Results

3.1. Flame Cone

Figure 2 shows the calculated cone shape flame stabilized on the burner rim. The cone is rather slender since the mixture flow velocity is much larger than the normal burning velocity. The left shows iso-lines of HCR (H2 consumption rate) in color, while the

![Fig. 2 Calculated cone-shaped flame shown by iso-lines of H2 consumption rate (left) and of temperature (right).](image)

![Fig. 3 Radial distributions of H2 mass fraction and consumption rate (upper) and temperature and heat release rate (lower), at 0.4 cm downstream of the burner exit, for 1D and 2D axisymmetric flames.](image)

![Fig. 4 Radial H2 (upper) and O2 (lower) concentration profiles at four axial positions. Solid circles show points at which H2 consumption rate takes its maximum.](image)
right shows iso-temperature lines. In Fig.3 the radial distributions of H2 mass fraction and HCR (upper), and of temperature and HRR (heat release rate) (lower), of the representative cone portion at 0.4 cm axial position, are shown as compared to those of a 1D flame. H2 decreases outward and the consumption rate takes a peak at a certain radial position corresponding to the flame cone. The coordinate of 1D flame is adjusted so that the positions of HCR peak should coincide with that of 2D axisymmetric flame. Although the cone is angled slightly, the radial distributions of H2 concentration and temperature, as well as the consumption rate and the heat release rate, of axisymmetric 2D flame appear very similar to those of 1D flame, and the 1D flame-like structure is established along the cone. It should be noticed that HRR is located upstream of HCR. Figure 4 shows the radial H2 and O2 concentration profiles of cone portion at 4 axial positions. The solid circles show the radial point at which HCR attains the maximum and the concentrations at that point. The distribution causes an outward diffusion of H2 molecules that reduces the H2 concentration of the mixture entering into the reaction zone. Please note that the H2 concentration on the axis decreases towards downstream. Outward O2 diffusion also takes place, but at a much slower rate. The H2 concentration at the HCR peak decreases towards downstream (upper), whereas O2 concentration increases slightly (lower).

The enlarged view of Fig. 5 shows details of the stream lines and iso-HCR (left) and HRR (right) lines in the vicinity of the tip. In this figure, radial distance is exaggerated by four times over axial distance to show the internal flame structure more clearly. The bold solid line represents the loci of the positions, where the radial distribution of HCR attains its maximum value. As is seen in the figure, the peak value of HCR, as well as that of HRR actually decreases toward the tip. It can also be seen that HRR peak occurs always in the upstream of HCR peak. The decrease of HCR towards downstream can be seen more clearly in the left of Fig. 6, where the variation along the HCR peak locus of temperature, HCR peak value, and mass fractions of involved species are shown. The right figure shows the result for the 2D plane flame without circumferential curvature, which will be described later. The abscissa represents the axial distance from the burner exit. The peak value of HCR decreases towards the tip. The temperature and H2O concentration remain almost constant. The H2 concentration decreases gradually, but O2 increases slightly. H decreases, whereas O and OH remain almost constant. In anyway, the flame structure does not remain uniform along the cone, and the deviation from the 1D flame becomes larger towards the downstream. Figure 7 shows the radial distribution of HCR through the five elementary reactions involved in H2 consumption, at the point 0.4 cm downstream of the burner exit (left), compared with that of a 1D flame (right). In both flames, the contribution of R3 reaction is the largest, followed by R2. The comparison reveals that the profiles are somewhat similar to those of the 1D flame, and here again we see that 1D-like flame structure is established. However, the R3 and R2 contributions are a little smaller in the 2D axisymmetric flame. Both reactions are H2-consuming and the consumption rates are proportional to H2 concentration. This figure explains why the peak of H2 consumption rate decreases downstream in
the 2D axisymmetric flame, that is, as is seen Fig. 4, the H$_2$ concentration of the mixture entering the reaction zone decreases downstream.

An additional 2D plane flame calculation has been done to see the flame structure without the effects of circumferential curvature, in the same way as [21] in which the laminar hydrogen premixed flame speed is measured and calculated. The calculation has revealed that in the 2D plane flame, there is the outward diffusion of H$_2$ molecules which reduces the H$_2$ concentration of the mixture entering into the reaction zone, in the same way as the axisymmetric flame. The lower figure of Fig. 6 shows that the non-uniform behavior is identical with that of axisymmetric flame, although the H$_2$ deficit is a little bit smaller in the plane flame.

To study further the effects of thermal diffusion, calculations were also carried out that neglected the thermal diffusion for H$_2$ and H. The comparison of the calculated radial H$_2$ and H concentration profiles, with the thermal diffusion and without it, has revealed that the thermal diffusion indeed accelerates the radial diffusion of H$_2$. On the other hand, the effect on H is not immediately apparent. With the thermal diffusion, the H profile remains almost the same, but the values become slightly smaller.

On the other hand, the reaction zone on the axis near the tip is shifted downstream considerably with the thermal diffusion. In addition the peak reaction rate is decreased. These findings appear to show the significant effect of thermal diffusion. However, further examination has revealed that the downstream shift comes mostly from the deceleration of the burning velocity of hydrogen-air premixed flame with the thermal diffusion as reported by Warnatz [22]. As the burning velocity becomes smaller, the flame cone becomes longer and the reaction zone on the axis is forced to shift downstream. In order to compensate for this change in the burning velocity for the case without thermal diffusion, the mixture velocity at the burner exit is changed to just 8 times the burning velocity, as is the case with thermal diffusion. Then it turns out that the downstream shift of reaction zone disappears. Next, to study further the effects of thermal diffusion on the non-uniformity of the HCR along the flame cone, the curves shown in Fig. 6 were calculated for the case without thermal diffusion and the result is shown in Fig. 8. Comparison with Fig. 6 reveals that the overall behavior of the HCR peak is very similar. In this sense, we may say that the thermal diffusion does not significantly affect the noteworthy feature of the flame cone.

3.2. Flame Tip Region

In this paper, the flame tip is defined as the position of HCR peak on the axis, and is located at around 1.2 cm position from the burner exit. The stream lines of Fig. 5 show that the mixture flow on the axis is forced to diverge and is decelerated as it approaches the flame tip, and is accelerated again after passing through the reaction zone. This behavior can be seen more clearly when we look at variations along the central axis in Fig. 9, where the axial velocity and mass flux on the axis are shown and are compared with those of 1D flame. In the figure, velocity...
is normalized by the burning velocity of 1D flame and mass flux is normalized by the mass burning velocity of the 1D flame. The mass flux of the 1D flame remains constant through the flame to give the eigenvalue mass burning velocity. On the other hand, in the 2D axisymmetric flame the mass flux increases slightly just upstream of the flame tip and then decreases very quickly, since the stream lines diverge and some of the mass flux that was originally on the axis flows away in the radial direction. As is seen clearly there are no definite mass burning velocities or burning velocities which can characterize the combustion on the axis. The original mass flux at the burner exit is 8, in the non-dimensional unit, and decrease to almost unity through the tip.

On the axis, the H₂ mass conservation equation is given by

$$\frac{\partial \rho Y_{H_2}^u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u v_{H_2}^{\text{dif}} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( \rho r v_{H_2} v_{H_2}^{\text{dif}} \right) + \dot{\omega}_{H_2} = 0,$$

where $u$ and $v$ are the axial and radial velocity components, $v_{H_2}^{\text{dif}}$ and $v_{H_2}^{\text{dif}}$ are the axial and radial diffusion velocities of H₂ including thermal diffusion effect, and $\dot{\omega}_{H_2}$ is the H₂ mass production rate. Other notations follow the common usage.

Figure 10 presents the variation along the axis of the respective terms of the above equation, as compared to that of the 1D flame. The contribution of chemical reaction remains very small in 2D axisymmetric flame. Figure 11 gives the magnitudes of the five terms integrated axially from the upstream burner exit to the downstream infinity. They give the following physical significances. The first term gives the inlet H₂ mass flow rate. The second axial diffusion term vanishes automatically by integration. The third and the fourth terms represent, the mass flow rate leaving axis by radial convection and by radial diffusion, respectively. The final fifth term represents the total mass consumption by chemical reactions. Each term is normalized by the normal mass burning velocity of the 1D flame. We now understand how the most of original H₂ mass flow is lost by outward radial diffusion and convection. Consumption by chemical reaction accounts for only around 1/18 of the original H₂ mass flow.

The flame tip region on the axis is surrounded by the hot cone portion, and the temperature in the preheat zone should decrease.
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On the axis the sensible energy equation is given by

\[ \frac{\partial h}{\partial x} + \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} + \sum_s \rho Y_s h_{s,\text{av}} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( \lambda \frac{\partial T}{\partial r} + \sum_s \rho Y_s h_{s,\text{av}} \right) + Q = 0, \]

where \( h \) and \( h_s \) are sensible enthalpies of the mixture and chemical species \( s \), respectively, and \( Q \) is chemical heat release, and small viscous dissipation term is excluded. Figure 12 compares the axial variation of respective terms in the above energy equation and the same figure for a 1D flame is shown for comparison. The large negative contributions of axial convection correspond to temperature rises in the axial direction, because the outgoing energy flux is larger than the incoming energy flux when the temperature rises in the control volume. In the 1D flame, the incoming mixture is preheated by the back heat diffusion from the downstream hot reaction zone. On the other hand, in the 2D axisymmetric flame it is mostly radial heat diffusion that contributes to heat up the incoming mixture, and we note that this heat supply from the outer cone is significant to keep the flame tip at this axial position. Then Fig. 13 gives the magnitudes of the respective terms integrated from the upstream burner exit to the downstream infinity, in the same way as in Fig. 11. In this figure, thermal conduction and enthalpy transfer by molecular diffusion are bundled together into the diffusion term, and each term is normalized by the sensible energy difference between unburnt and burnt mixture of 1D flame. The negative contributions of convections to the sensible energy of the mixture correspond to the temperature rise, here again. The figure reveals that this heat input is some two times the total heat released by chemical reactions on the axis, and that the heat supply by heat diffusion from the outer cone is indispensable to sustaining the reactions going on at the tip. In Fig. 14, HRR contribution profiles on the axis of six elementary reactions (upper) are shown as compared to those of the 1D flame (lower). In the upper figure, we notice that the greatest heat release is provided through R10. The contribution of R3 is smaller as compared to that of 1D flame, because of the \( \text{H}_2 \) deficit shown in Fig. 6.

4. Discussions

4.1. Flame Cone

We now understand that the local flame structure of the cone portion of the Bunsen flame does not remain uniform along the flow direction, but that the fuel consumption rate decreases towards downstream. We think that the observed decrease of HCR comes simply from the decrease of \( \text{H}_2 \) concentration entering into the cone. The present study has revealed that this is caused by the outward molecular diffusion of \( \text{H}_2 \) in the original mixture. Although \( \text{O}_2 \) is also diffused, \( \text{H}_2 \) is much more mobile
leading to an appreciable H₂ deficit in the mixture entering into the reaction zone of the downstream cone portion. Some further discussions must be made regarding this effect. The equivalence ratio of the mixture coming into the reaction zone is decreased in the downstream direction. This may lead to an argument that in the downstream cone portion the rates of chemical reactions should be reduced because of the decrease in equivalence ratio, and hence of the flame temperature. However, Fig. 6 reveals that the temperature at the HCR peak remains almost constant. It is not the deficit of equivalence ratio, but of H₂ concentration itself, which causes the deceleration of HCR through the R3 and R2 elementary reactions. While the R3 reaction contributes somewhat to heat release. As is seen in Fig. 14, its contribution to the total heat release of 2D axisymmetric flame is rather small compared to that to H₂ consumption rate. Then the effect of the H₂ deficit in the mixture coming into the flame cone should not be so significant to HRR as compared to that to HCR. This explains why the temperature at the peak remains almost constant in Fig. 6. The peculiar behavior of H₂ molecule described above combined with R3 and R2 elementary reactions brings about the non-uniformity of HCR, but temperature is little affected, in the flame cone.

Another problem to be discussed is the effect of flame circumferential curvature. In Fig. 6, HCR peak value decreases towards tip not only for the axisymmetric flame but also for the plane flame without flame circumferential curvature. The result suggests that the preferential diffusion mechanism is not essential in this flame. The present study has revealed that the decrease is caused by the H₂ deficit due to the mobile H₂ diffusion. The present numerical study has also shown that thermal diffusion does not significantly affect the Bunsen flame structure. One problem with thermal diffusion is that there are a variety of formulae to represent the diffusion effect, and we do not know, at this stage, which is the best one to adopt. In the present study, we simply follow the formula developed by R. J. Kee et al. [17].

4.2. Flame Tip Region

We now understand that the flame tip structure of the Bunsen burner flame is fundamentally two-dimensional, and the mixture mass flux coming into the tip is largely reduced by flow divergence and outward diffusion, as is seen in Fig. 9. This reduced mass flow rate is consumed by chemical reactions with an aid of inward heat diffusion from the outer cone. The flow on the axis is enclosed by the flame cone, and there is the radial temperature distribution increasing outward to cause the radial heat diffusion inward. It is this radial heat diffusion from the outer cone, rather than axial diffusion from the downstream hot burnt gases, differently from 1D normal flame that heats the incoming mixture. This tip behavior cannot be explained in terms of any of the extended 1D flame theories. Neither the Lewis number effect nor the strain and curvature effect on the burning velocity of a 1D flame can be applied. In addition, our complementary study to find the effects of burner diameter has revealed that the effect of curvature does not follow the prediction of the conventional preferential diffusion mechanism [8,10]. The observed dependence on the burner diameter is rather complicated and further studies must be made to understand the behavior.

Figure 9 has revealed that there is no mass flow rate to define the unique mass burning velocity, in contrast to the 1D normal flame. In such situation, there does not exist any unique relation between the burning velocity and flame properties, and therefore any attempt to explain the flame properties change in terms of the burning velocity modification cannot be successful [6]. Furthermore, we wonder if the tip itself can be called a kind of the premixed flame. Because the tip is not self-sustained any more, and the mixture is burning with a strong aid of the heating by the outer flame cone. We must develop a 2D theory based on this finding to describe the burning process at the tip. Further studies must be continued to understand the detailed burning process of the tip. The effects of equivalence ratio and mixture flow velocity should be other interesting topics, and they should be examined in the next study, as related to the tip opening.
5. Conclusions

Precise numerical study has revealed the detailed 2D axisymmetric flow, temperature and concentration fields of the stoichiometric hydrogen-air Bunsen flame. The chemical reactions along the cone portion do not remain uniform. The H₂ consumption rate decreases towards downstream. This is caused by the decrease of H₂ concentration of the mixture coming into the cone through the outer diffusion of mobile H₂ molecules combined with the slowdown of the R3 and R2 elementary reactions. In this decrease the preferential diffusion mechanism due to the flame circumferential curvature is not essential. It is also clarified that the flame structure at the tip is fundamentally two-dimensional, and that the mixture coming into the tip on the axis is largely reduced by the outward radial convection and diffusion before entering into the reaction zone, and the remaining mixture can continue combustion reactions by an aid of radial heat diffusion from the outer flame cone. The result raises a serious question if the tip can be called a part of the premixed flame. The thermal diffusion does not seem to affect the flame structure significantly.

In this study we investigated the case of stoichiometric mixture injected at a velocity of 8 times the normal burning velocity of 1D flame. The flame structure, especially the tip structure, depends on the equivalence ratio and the flow velocity of the mixture. We will discuss such issues in the next study related to the tip opening.

Acknowledgments

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References