The characteristics of triple flames in a hydrogen–air mixing layer are studied using direct numerical simulation with detailed chemistry. Triple flames are initiated by imposing a temperature ignition source in the center of a scalar mixing layer of nonuniform thickness, thereby forming a pair of freely propagating triple flames. Two different fuel streams are studied: pure hydrogen and hydrogen diluted with nitrogen. During the ignition stage, the initial ignition runaway is followed by a secondary peak as the ignition kernel transitions to a triple flame, consistent with previous observations. For both diluted and undiluted cases, the triple flame structure exhibits more similarity with a diffusion flame than with a premixed flame, such that the triple point, defined as the location of maximum heat release, is always in the proximity of the stoichiometric mixture fraction line. Similar to a previous study of methanol–air triple flames, the enhancement in the stabilization speed is attributed mainly to flow divergence, and its value is proportional to the square root of the density ratio across the flame. In the undiluted case, however, the asymmetric flame structure results in distinct locations where the stabilization speed and the displacement speed are maximum. The effect of unsteady strain rate is also studied by imposing a pair of vortices on the propagating triple flames. The negative strain rate results in the collapse of the premixed flame branches onto the diffusion flame, forming an edge flame structure. Excessive compressive strain and curvature at the triple flame tip leads to a negative displacement speed. A mixture fraction/temperature parameterization is shown to be useful in representing the structure of a triple flame subjected to unsteady strain rate. © 1999 by The Combustion Institute

INTRODUCTION

The stabilization mechanism of lifted flames in turbulent jets or mixing layers is still one of the unresolved issues in turbulent combustion. At the flame stabilization point the local flame structure may involve partial premixing of reactants and interaction with unsteady aerodynamic strain arising from a wide range of turbulent eddies. Understanding the dynamics of these flames is needed for appropriate description and prediction that are useful in the development of practical combustion devices.

Through a number of recent studies since its inception by Liñán and Crespo [1], the triple flame has emerged as a potential canonical edge-flame structure to describe the flame stabilization mechanism in a partially premixed mixture. A triple flame is comprised of a curved premixed front spanning rich and lean compositions which propagates along the stoichiometric mixture fraction line. Excess fuel and oxidizer that survive through each branch of the premixed flames form a trailing diffusion flame behind the stoichiometric point. The intersection of the three branches is termed the “triple point” in this paper. The propagation speed of the triple flame is different from that of the stoichiometric premixed flame and depends on various parameters including the Lewis number [2, 3] and mixture fraction gradient [4, 5]. The effect of heat release has been studied by Retsch et al. [6], in which a scaling law was proposed for the flame speed with respect to upstream flow conditions. Ghosal and Vervisch [7] extended the asymptotic analysis by Hartley and Dold [4] to include the effect of finite heat release rate. Further experimental measurements [8, 9] have confirmed that the local flow velocity at the stabilization point is indeed of the order of the laminar flame speed. More recently, Ko and Chung [10] have experimentally observed that the displacement speed of a methane–air triple flame is several times larger than the laminar flame speed. These results suggest that the triple-flame structure has an intrinsic stabilization mechanism, whereby the upstream flow velocity is reduced to the laminar flame speed by streamline divergence behind the curved triple flame front. A further consequence of heat...
release is the modification to the mixing thickness ahead of the flame.

Triple flames may also play an important role in the ignition and further propagation of flames in a partially premixed system, such as in a diesel engine in which fuel and air are not fully mixed prior to ignition. Domingo and Vervisch [11] have demonstrated the relevance of triple flames in their direct numerical simulation (DNS) of turbulent compression ignition, in which the flame spread from the ignition point was via the propagation of triple flames along the stoichiometric contours in the turbulent scalar field.

Most previous studies including asymptotic and numerical analysis employed a simple global-step chemistry. Although the flow-divergence effect, which is the primary stabilization mechanism, can be captured by considering only thermo-fluid dynamic aspects of the flame, better understanding of the detailed structure and chemical response can provide further insight towards a realistic picture for practical flames. A direct simulation of a methanol–air triple flame has been performed by Echekki and Chen [12], in which the detailed flame structure and the effects of heat release and differential diffusion on the flame propagation have been identified. It was found that differential diffusion of hydrogen amplified by the curvature of the flame tip contributes to the enhancement of the flame speed through chemical effects. Plessing et al. [13] have also investigated the stabilization mechanism and structure of methane–air triple flames using reduced chemistry.

In the present paper we consider triple flames in a hydrogen–air mixing layer for an idealized configuration. This study is motivated by several factors. First, for most hydrocarbon triple flames CO and H₂, intermediates from the rich premixed flame branch, are the stable fuels that burn in the diffusion flame [12]. On the other hand, in a hydrogen–air mixture the fuel species, H₂, survives through the rich premixed flame branch. Therefore, the hydrogen–air system provides a more prototypical flame structure that can be compared with existing theoretical and computational results with simple chemistry. Second, it is well known that the laminar flame speed of a homogeneous hydrogen–air mixture is maximum at an equivalence ratio greater than unity. Therefore, it may be anticipated that the triple point, which governs the overall propagation speed and thus the stabilization mechanism, may be located on the rich side of the stoichiometric line. This unique characteristic of hydrogen–air flames may lead to propagation and structural differences compared to hydrocarbon flames. Finally, for homogeneous premixed flames, the hydrogen–air system exhibits the most significant effect of preferential diffusion due to the high diffusivity of hydrogen. This effect may be amplified at the highly curved triple flame tip, and may affect the local propagation. Furthermore, using the temperature–mixture fraction parameterization suggested by Echekki and Chen [12], the effect of unsteady flow straining on the triple flame structure is studied by the interaction of a triple flame with a pair of vortices.

CONFIGURATION AND NUMERICAL METHOD

The full compressible Navier-Stokes, species and energy equations for a reacting gas mixture are solved using a fourth-order Runge-Kutta method for time integration and an eighth-order explicit spatial differencing scheme [14]. To ensure sufficient spatial resolution, the energy spectrum of flow and all the species are continually checked throughout the simulation. Typically, the grid size is chosen such that the energy contained in a wavenumber range of \( k \Delta/2 \pi > 0.5 \) is less than 0.1% of the total energy of each variable, where \( k \) is the wavenumber and \( \Delta \) is the grid size. A detailed hydrogen–air mechanism with 9 species and 38 reversible reactions [15] is adopted. The molecular viscosity is temperature-dependent \( (\sim T^{0.7}) \) and the Prandtl number is taken to be 0.708. The mass diffusion coefficients for individual species are determined by constant Lewis numbers given as

\[
Le_{H_2} = 0.3, \quad Le_{O_2} = 1.11, \quad Le_O = 0.7,
\]

\[
Le_{OH} = 0.73, \quad Le_{H,O} = 0.83, \quad Le_{H} = 0.18,
\]

\[
Le_{HO_2} = 1.10, \quad Le_{H_2O_2} = 1.12.
\]
The velocity and time scales are normalized by acoustic scales for air at 300 K, such that the reference velocity and time scales are $u_r = 347.9 \text{ m/s}$ and $t_r = L_r/u_r = 12.95 \mu\text{sec}$, if the reference length scale is set to $L_r = 4.5 \text{ mm}$.

A schematic of the problem configuration is shown in Fig. 1. The computational domain is two-dimensional with dimensions of $7.2 \text{ mm} \times 3.6 \text{ mm}$, in which $1001 \times 501$ grid resolution is used. A hydrogen–air mixing layer at the ambient condition (300 K, 1 atm) is initially imposed with a mixing thickness which varies continuously from 2.5% to 50% of the shorter domain length. Two different concentrations are chosen for the fuel stream: (a) pure, undiluted hydrogen, and (b) hydrogen diluted with 50% nitrogen by volume. The oxidizer stream is chosen to be air. Nonreflecting boundary conditions are imposed at all boundaries.

To initialize the triple flames, a concentrated Gaussian temperature field of the form:

$$
T(x, y) = T_0 + (T_{\text{max}} - T_0) \cdot \exp\left[-\frac{(x-x_c)^2}{\delta^2}\right] \exp\left[-\frac{(y-y_c)^2}{\delta^2}\right]
$$

is imposed at the center of the mixing layer at $x = x_c$ and $y = y_c$. In this study, $T_0 = 300 \text{ K}$ and $T_{\text{max}} = 3000 \text{ K}$, while the width of the initial temperature profile, $\delta$, is set to be a small value of $\delta = 0.05 \ L_r$, in order to ensure that the effect of the artificial ignition source vanishes sufficiently fast (see Appendix). Due to the high temperature of the ignition source, ignition occurs rapidly and a pair of triple flames develop and propagate along the stoichiometric mixture fraction line in both directions. No attempt was made to stabilize the flame in the domain.

The simulation was performed on a Silicon Graphics Origin 2000 parallel computer. Each of the two concentration cases was computed up to $50 \ t_r \approx 0.65 \ \mu\text{sec}$, at which time the leading edge of the triple flames approaches the end of the domain. Using approximately 20 R10000 processors on average, each case required approximately 1 month of continuous run time.

One of the important parameters to characterize a partially premixed system is the mixture fraction variable. While there is no unique definition of the mixture fraction for multicomponent systems due to differential diffusion, the formula suggested by Bilger [16] captures the stoichiometric lines properly. The mixture fraction, $\xi$, is defined as a linear combination of the elemental mass fractions, $Z_H$ and $Z_O$:

$$
\xi = \frac{1/2 Z_H W_H + (Z_{O,O} - Z_O) W_O}{1/2 Z_H W_H + Z_{O,O} W_O},
$$

where the subscripts $F$ and $O$ respectively denote the fuel and oxidizer streams, and $W_H$ and $W_O$ are the molecular weights of H and O atoms. For the mixtures used in this study, the stoichiometric condition is at $\xi_{st} = 0.3042$ for the diluted case and 0.0285 for the undiluted case.

**IGNITION STAGE**

We first examine the initial transient behavior during ignition and formation of the triple
flames. Figure 2 shows a time sequence of heat release isocontours during the development of the triple flames from ignition, for the diluted fuel stream case. With an initial peak temperature of 3000 K in the ignition source, ignition occurs rather rapidly, at $t/\tau_r \approx 0.2$. Since heat release in a hydrogen–air system is dominated by the recombination step, $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$, the heat release is initially maximum on the air side (right half of domain) where $\text{O}_2$ is more abundant. Subsequently, as shown in Fig. 2, the location of maximum heat release bifurcates, with each of the peaks aligning with the stoichiometric mixture fraction line in the vertical direction.

Figure 3 further shows the history of maximum temperature and species mass fractions during the ignition stage. As expected in the hydrogen system, the ignition event is characterized by an initial build-up of $\text{HO}_2$ radical followed by the development of a radical pool consisting of $\text{H}$, $\text{O}$, and $\text{OH}$. We note that there exists a double-peaked response of most of the major radicals: the first peak due to ignition runaway followed by a second peak as the ignition kernel completes its transition to a triple flame. Similar behavior has been observed in simple-chemistry results by Domingo and Vervisch [11], in which the double-peaked be-

Fig. 2. Time sequence of the heat release isocontour during ignition and development of the triple flames. Time is normalized by the acoustic time scale, $\tau_r = 12.95 \ \mu\text{sec}$.

Fig. 3. Maximum temperature and selected species mass fractions as a function of time during the ignition stage, for the diluted case.
behavior has been suggested as an indicator of the existence of triple flames in the ignition of turbulent mixtures.

STRUCTURE OF THE TRIPLE FLAME

Once ignited, a pair of triple flames propagate in each of the two directions approximately along the stoichiometric mixture fraction line. A generic flame structure is first described using the data for the diluted case which shows a more symmetric mixing structure. The results of the undiluted case are then presented in a later section to highlight the distinct features of hydrogen–air triple flames.

Figure 4 shows the reactants and intermediate species profiles for the upper half of the computational domain for the diluted case after the ignition transient has vanished and the triple flame is established ($t/\tau_r = 40$). It is clearly seen that, unlike in hydrocarbon flames, excess in the original fuel, $H_2$, diffuses through the rich premixed flame and reacts at the stoichiometric line of the diffusion flame with $O_2$ that has survived through the lean premixed flame. As in homogeneous premixed flames, the leading edge of the premixed flame envelope, for both lean and rich branches, is adequately represented by the $HO_2$ layer that is formed in the low-temperature preheat zone via the recombination reaction, $H + O_2 + M = HO_2 + M$. The $HO_2$ layer is then followed by other major radical species, $H$, $O$, $OH$, and by product, $H_2O$. The production of $OH$ radical is mainly due to the branching step, $O_2 + H = O + OH$, such that the peak in $OH$ concentration is located on the lean side of the stoichiometric line. On the other hand, $H$ atom, produced mainly by the consumption of $H_2$ via $H_2 + OH = H_2O + H$ and $H_2 + O = OH + H$, favors the rich side. As observed in the methanol–air triple flame [12], the relatively slow recombination process of $OH$ causes its maximum concentration to occur further downstream in the diffusion flame, unlike $H$ and $O$ atoms which peak near the leading edge of the triple flame.

Figure 5 shows the corresponding reaction and heat release rate isocontours for the data field shown in Fig. 4. It is noted that the isocontours of the reaction rate for $H$ atom best capture the three distinct branches of the triple flame structure. While the reaction rate profiles corresponding to $O_2$ and $H_2O$ also reveal the triple flame structure, the enhanced $O_2$ consumption and $H_2O$ production on the lean side, combined with the shift in $\xi_{st}$ to the lean side due to the high diffusivity of hydrogen, render the lean premixed flame branch and the diffusion flame less distinguishable from each other. The maximum value of the heat release occurs near the leading edge, slightly shifted toward the lean side. This reflects the fact that the major exothermic reaction step, $H + O_2 + M = HO_2 + M$, is most prominent in the lower temperature preheat zone.

Therefore, unlike a triple flame described by a global single step for which the maximum heat release and reactant consumption coincide at the leading edge of the stoichiometric line.
thereby constituting a well-defined triple point, in a hydrogen–air triple flame the exact definition of the triple point is ambiguous since the peaks of heat release and H atom production rate, respectively, are located on the lean and rich sides of the stoichiometric line. Consistent with previous studies [12], the triple point in the present study is defined as the location at which the maximum heat release occurs.

PROPAGATION SPEED OF THE TRIPLE FLAME

First, it is of interest to identify the homogeneous premixed flame speeds for various mixture conditions as reference quantities for analyzing the triple flame speed. The laminar flame speed for mixtures given by the formula

$$\phi[(1 - \alpha)H_2 + \alpha N_2] + 0.5(1 - \alpha)$$

$$\cdot [O_2 + 3.76N_2]$$

is computed for various equivalence ratios, $\phi$, and fuel stream dilutions, $\alpha$. Figure 6 shows the laminar flame speed of the diluted ($\alpha = 0.5$) and undiluted ($\alpha = 0$) mixtures as a function of the equivalence ratio. The open symbols denote the results obtained from PREMIX [17] using mixture-averaged transport properties, and the solid symbols denote the DNS results with simplified transport. The simplified transport results capture the overall trend, e.g., the equivalence ratio at the peak laminar flame speed, with an error in the flame speed of less than 10%. The maximum flame speed occurs at $\phi = 1.5$ and 1.8 for the diluted and undiluted cases, respectively. The actual values of the laminar flame speed and the flame time based on the thermal thickness, $\ell_{fl}$, are

$$S_L^0 = 1.39 \text{ m/sec, } \tau_{fl} = S_L^0 / \ell_{fl} = 21.67 \tau_r$$

= 0.280 msec, for the diluted case,

$$S_L^0 = 2.43 \text{ m/sec, } \tau_{fl} = S_L^0 / \ell_{fl} = 10.93 \tau_r$$

= 0.142 msec, for the undiluted case.

For either case, the stoichiometric flame speed and the density of the corresponding fresh
mixture at 300 K is used to normalize the results. The solutions are integrated over two flame times, based on the flame speed and thermal thickness of the reference laminar flame.

The propagation speed of the triple flame is obtained by evaluating the displacement speed of the flame front relative to the local flow velocity. The density-weighted displacement speed, $S^*_d$, determined from an isoline of species $i$ is defined as [6, 12]

$$ S^*_d = \frac{\rho S_d}{\rho_u} = \pm \left[ \frac{w_i}{\rho_u |\nabla Y^i|} + \frac{\partial}{\partial x_j} \left( \frac{\rho D_i \partial Y^i}{\rho_u |\nabla Y^i|} \right) \right] $$

where $\rho_u$ denotes the density of the unburnt mixture, and $D_i$ is the local mass diffusivity of species $i$. The sign in Eq. 4 is positive for products and negative for reactant species. The density-weighted formulation minimizes dilatational effects on the displacement speed across the flame thickness [12], and is used as a measure of the effects of stretch/curvature/prefential diffusion on the flame speed relative to the laminar flame speed.

Since the flame has finite thickness in which various layers of individual species exist at different locations, there is ambiguity as to the choice of a particular isoline used to evaluate the displacement speed. One choice is to define a species isocontour that is aligned with the maximum heat release rate. Since neither reactant, H$_2$ or O$_2$, properly represents the entire envelope of the triple flame front due to the partially premixed composition field, we choose an isoline of the product concentration, $Y_{H_2O}$. As shown in Fig. 7 for the diluted case, the isoline $Y_{H_2O} = 0.03$, corresponding to 10% of its maximum downstream value, represents the maximum heat release isocontour and the overall shape of the triple flame reasonably well.

In addition to the displacement speed relative to the local flow velocity, a quantity of practical interest is the flame speed relative to the far-upstream gas velocity. This stabilization speed, $V_f$, is evaluated as [12]

$$ V_f = (S_d + u \cdot n) + u_u, $$

where $u$ is the local gas velocity vector and $u_u$ is the upstream flow velocity. In this study of freely propagating triple flames, $u_u$ is zero by definition and thus $V_f$ corresponds to the lab-frame velocity. The flame normal vector, $n$, is defined as

$$ n = \begin{cases} \frac{\nabla Y^i}{|\nabla Y^i|} & \text{for reactants,} \\ -\frac{\nabla Y^i}{|\nabla Y^i|} & \text{for products,} \end{cases} $$

such that $n$ is always directed towards the direction of propagation. As long as the triple flame structure propagates as a single identity, $V_f$ remains constant through the flame, irrespective of thermal expansion effects.

In the earlier ignition stage, say up to $t/\tau_r = 5$ (see Fig. 2), the propagation speed of the flame...
is altered by the initial hot temperature ignition source. In addition, the growing “flame ball” creates an induced velocity field ahead of it, thus further contributing to an enhanced propagation speed. In the results presented herein, however, these initial transients are found to disappear quickly, such that each triple flame reaches a freely propagating state during a substantial portion of the total computation time.

Although not shown here, we have confirmed that the pressure in the region between the two triple flames reaches the ambient value for most of the solution fields in the later stage, hence suggesting that the mutual interaction of the two triple flames is negligible. In the Appendix, numerical fidelity of the solutions and the effect of the initial ignition source are validated by a one-dimensional simulation. The additional test simulation presented in the Appendix further confirms that the flame-ball effect is indeed insignificant.

Figure 8 shows the computed speed and velocity profile along the flame normal through the triple point, which is approximately along the vertical line following the stoichiometric line, for the lower flame segment shown in Fig. 7. The origin of the normal is the location of maximum heat release ($Y_{H_2O} = 0.03$). The H$_2$O profile is also presented in Fig. 8 to indicate the location of the flame. It is observed that the velocity normal to the flame, $u_n = -u \cdot n$, decreases as the flow approaches the flame due to flow divergence, consistent with the results by Ruetsch et al. [6], and then increases within the flame due to thermal expansion. The displacement speed, $S_d$, also shows a similar increase through the flame. It is noted that $S_d$ values are meaningful only within the thermal thickness where significant species mass fraction gradient exists, as denoted by the shaded area in Fig. 8. As given by Eq. 6, the stabilization speed, $V_f$, is the difference between $S_d$ and $u_n$, which essentially remains constant across the flame. For this case $V_f/S_d = 2.41$, which is very close to the square root of the density ratio, $\sqrt{\rho_f/\rho_b} = 2.42$. Although the agreement appears to be excellent, it should be noted that there is a little ambiguity in identifying the most relevant density ratio. That is, while the scaling relation suggested by Ruetsch et al. [6] is based on the assumption that density is uniform in the fresh mixture, in the present hydrogen–air mixture a significant density variation exists across the mixing layer due to the large difference in the density of hydrogen and air. Here, the density ratio is determined from the maximum and minimum density along the stoichiometric line.

The increase in the stabilization speed can be attributed to two effects: (a) flow divergence occurring in the preheat zone, and (b) the local flame speed variation due to the combined effects of stretch, curvature, and preferential diffusion of various species. In order to distin-
To distinguish between these effects, the density-weighted displacement speed, \( S^* \), is computed along the flame normal as shown in Fig. 8. At the triple point, \( S^*_T = 0.987 \), implying that the effect of preferential diffusion of hydrogen, combined with the curvature at the triple point, is of little significance in the propagation speed variation. The contribution to the \( V_f \) enhancement is thus almost entirely attributed to the fluid-dynamic effect. This result is similar to observations made in a methanol–air triple flame [12], where the chemical enhancement to the flame speed was found to be small. The result may also be attributed to the fact that the effect of curvature at the triple point is not significantly large, since the radius of curvature is approximately twice the reference thermal thickness, \( \ell_f \), and the triple point is near the stoichiometric condition. Therefore, for the particular triple flame configuration studied here, it appears that preferential diffusion is no more pronounced for the hydrogen–air mixture than for the methanol–air mixture. In other words, the “Lewis number effect” is almost as negligible for the hydrogen mixture as it is for the methanol mixture which is expected to be thermodiffusively neutral.

Figure 9 shows the temporal variation of various flame speeds for the two triple flames for the diluted mixture. All of the quantities are evaluated at the point of maximum heat release along the \( Y_{H_2O} = 0.03 \) contour line. Initially, higher flame speeds are induced by the high-temperature ignition source and by the flame-ball effect, and subsequently approach a constant value after approximately one flame time \( (t \approx 24 \tau_r) \). The temporal behavior is qualitatively similar to recent experimental results by Ko and Chung [10].

The effect of the mixing layer thickness is also demonstrated in Fig. 9. It is shown that the triple flame propagating toward the wider mixing layer has a slightly higher stabilization speed, \( V_f' \), than that toward the narrower mixing layer. Furthermore, it is clearly seen that such difference is mainly due to the variation in \( u_n \), implying that a wider mixing thickness creates more significant flow redirection effect, consistent with earlier findings [6]. The local displacement speed, \( S_d \), as well as the density-weighted displacement speed, \( S^*_d \), show negligible difference for the two triple flames, with the values very close to the laminar flame speed of the stoichiometric condition.

Despite the large variation (a factor of 20) in the mixing layer thickness based on their far-upstream values, the difference in \( V_f' \) between the two triple flames is rather small (less than 10%). It appears that, in the absence of external forcing (such as flow shear or straining) to maintain the mixture fraction gradient, the downstream thermal expansion causes the mixing layer to spread out, rendering the triple flames less sensitive to the far-upstream mixing thickness. This result contrasts with previous experimental observations [10] in which the flame speed changes nearly twofold for a change in the mixture fraction gradient by an order of magnitude. It is not clear, however, whether the far-upstream mixing thickness in the present simulation can be directly translated into the mixture fraction gradient reported in the experiment. A careful consideration is needed on this issue.

**COMPARISON WITH THE UNDILUTED FUEL STREAM CASE**

In the previous sections, the structure and propagation characteristics of a hydrogen–air triple flame diluted with nitrogen by 50% volume have
been studied. The purpose of dilution is to achieve a triple flame that is more symmetric with respect to the stoichiometric mixture fraction line, thus allowing for clearer visualization of the structure. While the triple point structure exhibits characteristics closer to a diffusion flame rather than a hydrogen premixed flame, i.e., without pronounced effect of preferential diffusion or the shift of the triple point towards the rich side of the mixing layer, it may be argued whether such observations are attributable to the effect of fuel stream dilution which might attenuate the hydrogen flame characteristics. To assess this point, a second simulation is performed, identical to the configuration shown in Fig. 1, except that pure hydrogen is used in the fuel stream ($\alpha = 0$).

Figure 10 shows the heat release isocontours for the undiluted triple flame, at $t/\tau_r = 18$. Due to the increased propagation speed, the undiluted triple flame develops faster than the diluted case. Since the stoichiometric mixture fraction is shifted further towards the oxidizer side in this case ($\xi = 0.0285$), the triple flame structure is grossly asymmetric with respect to the stoichiometric line, such that the flame normal line through the triple point (maximum heat release point) is not as well-aligned with the stoichiometric line as in the diluted case (compared with Fig. 7).

Nevertheless, the overall structure of the triple point and the three branches shown in Fig. 10 appear to be similar to the diluted case, i.e., the triple point is still in the proximity of the stoichiometric line. The main qualitative difference is that the location of maximum heat release occurs slightly on the rich side of the stoichiometric line, rather than on the lean side as shown for the diluted case in Fig. 7. Although the heat release is still dominated by the three-body recombination reaction and thus should bias the lean side of the mixture, the lower specific heat of hydrogen compared to nitrogen causes the heat release peak to shift towards the richer side.

Unlike the diluted case, however, it is remarkable to observe that the local maximum of $S^*_{d}$ and $V_f$ occur at different locations along the 10% product mass fraction isocontour, as indicated by the arrows in Fig. 10. As the stoichiometric mixture fraction line is shifted further into the oxidizer side ($\xi_{st} = 0.0285$), due to the asymmetry of the triple flame, the location of the maximum flow redirection effect does not necessarily align with the stoichiometric mixture fraction line on which maximum heat release and displacement speed occur. To demonstrate this more clearly, Figs. 11 and 12 respectively show the temporal variation of various speeds at the locations of maximum $S^*_{d}$ (the triple point) and maximum $V_f$. Figure 11 shows that the maximum displacement speed at the triple point ($S_{d}$ or $S^*_{d}$) remains almost constant and the two

![Figure 10](image-url)
triple flames exhibit $S_d^*$ values very close to each other. As for the undiluted case, the difference in $V_f$ for the two triple flames propagating towards different mixing thickness is mainly due to the flow redirection effect represented by $u_n$. While $u_n$ at the triple point tends to approach a constant value (Fig. 11), the actual minimum value of $u_n$ continues to decrease, leading to a continuous increase in the maximum $V_f$ (Fig. 12). This result implies that the triple point and the actual leading edge of the triple flame may not coincide for some mixtures, and thus careful definition is needed for consistent comparison with experiments.

**INTERACTION OF TRIPLE FLAMES AND VORTICES**

To simulate the effect of unsteady straining on the structure and propagation of an edge flame, the interaction between a pair of counterrotating vortices and a laminar hydrogen–air triple flame is studied. The counterrotating vortices produce a strong compressive strain rate at the triple flame tip as it is pinched by the vortex pair, followed by a decrease in extensive strain rate along the stoichiometric line. This canonical flame/flow interaction is meant to simulate the strain field that an edge flame would encounter as it propagates upstream into a partially premixed region at the base of a lifted turbulent diffusion flame.

A vortex pair of a single strength and size are considered in the present study, although further investigation of the relevant vortex/flame parameter range is in progress. The solution field at $t/\tau_r = 15$ corresponding to the diluted case is restarted with a pair of counterrotating vortices just upstream of each triple flame. The azimuthal velocity profile of the vortex has the form:

$$u_\theta(r) = \frac{\beta \sigma^2}{2 \pi r}[1 - e^{-\sigma^2/r^2}],$$

where $r^2 = (x - x_c)^2 + (y - y_c)^2$ if the vortex is centered at $(x_c, y_c)$, and $\sigma$ is the nominal vortex radius. This is a modified form of the Oseen’s vortex with more rapid velocity decay. The azimuthal velocity has a maximum at $r = 0.9\sigma$, and $\beta = 0.9833$ is used to normalize the velocity with the maximum value. The direction of the vortex pair is such that the triple flame tip is pulled into the channel between the vortices. The ratio of the peak tangential velocity of the vortex and the laminar flame speed, $u_{\theta,\text{max}}/S_L^0$, is taken to be 14.3, the ratio of the vortex diameter, $\sigma$, to the laminar flame thickness is 1.9, and the separation between the centers of the two vortices is 1.5 $\sigma$. 

Since the propagation of the triple flame is due to the premixed nature of the flame, flame stretch may be used in quantifying the effect of unsteady strain rate on propagation than scalar dissipation rate. Flame stretch is represented by the Karlovitz number, 

$$K_a = \kappa \delta / S_L^0,$$

where the dimensional stretch, $\kappa$, is expressed as the sum of tangential strain rate, $a_T$, and a curvature term [18]

$$\kappa = a_T + S_\theta \nabla \cdot n. \quad (9)$$

Figures 13–15 compare the heat release, and reaction rates of H and H$_2$ for the field prior to vortex interaction and at $t = 10\tau$, when the triple flame tip is most stretched. The flame stretch at the tip is attributed primarily to curvature/propagation effects, leading to a curvature Karlovitz number, 

$$K_{a_c} = S_\theta \nabla \cdot n\delta / S_L^0,$$

of $-25$. By comparison, the local strain Karlovitz number, $K_{a_s} = a_T \delta / S_L^0$, is $-9$. After $t = 10\tau$, the pair of vortices drifts further away from the flame tip, so the triple flame recovers to the unstrained state.
Heat release is produced by production of HO$_2$ which occurs at the leading edge of the premixed branches. The net effect of unsteady straining by the vortices is the pinching of the premixed branches at the leading edge of the triple flame. This creates a highly curved triple flame, and H atom which is produced behind the premixed flame cannot diffuse upstream into this highly curved region. As a consequence, production and consumption of HO$_2$, which depends on the presence of H atom at the leading edge of the triple flame, is reduced. As shown in Fig. 13a prior to straining, the maximum heat release occurs slightly on the lean side of the stoichiometric line. For the strained case (Fig. 13b), the location of maximum heat release is shifted further into the lean premixed flame branch. The reason for this shift is that the peak H radical consumption is shifted toward the lean limit, as shown in Fig. 14. Radical consumption at the highly curved tip is negligible since H atom concentration, whose maximum is located behind its consumption layer, is defocused at the highly curved triple flame leading edge. While the local curvature is small in both the lean and rich branches, consumption rate of H atom is larger on the lean side due to the abundance of O$_2$. It is found that the maximum heat release for the strained case is 20% lower than for the unstrained case as a result of a decrease in the production rate of HO$_2$ at the leading edge of the triple flame, which depends on the ability of H atom to diffuse to the leading edge.

Fuel consumption is enhanced in the triple point region due to the differential diffusion of hydrogen towards the radical production layer, which is amplified in the presence of curvature effects at the flame tip. The center of curvature at the triple region is in the burnt gases, thereby focusing hydrogen towards its consumption layer. A 35% increase in the peak production rate of H atom is observed for the strained case. Consequently, fuel and oxidizer consumption rates shown in Fig. 15b are found to be enhanced by as much as 40%. Furthermore, as a result of the extensive strain rate along the stoichiometric mixture line, the consumption of fuel and oxidizer in the diffusion flame are also enhanced relative to the unstrained case, making the transition in consumption and heat release rates more gradual between the premixed and diffusion flame branches. It is noted that, in Fig. 15b, under the influence of large unsteady straining, the lean and rich premixed branches of the triple flame collapse, forming an “edge flame,” with the peak in the fuel consumption rate occurring at the triple point region and decreasing along the stoichiometric line.

To examine the variation of the flame speed during unsteady straining, $S_{d}^*$ based on the $Y_{H_2O} = 0.03$ isoline is monitored at the tip of the strained triple flame. We remark that, due
to the highly transient local flow field, a direct comparison of $V_f$ is of little relevance to the actual stabilization speed of the flame unless it is averaged over a long period of time. Figure 16 shows the variation in $S^*_d$ and the curvature, which is the main component of flame stretch, during the interaction. During a substantial period of the interaction, a negative displacement speed is observed due to the excessive positive curvature and compressive strain [19, 20]. After the interaction, the triple point recovers to a positive displacement speed.

As a final note, we remark that the triple flame structure can be systematically mapped into a phase space using two parameters, temperature and mixture fraction which, respectively, represent the degree of reaction and mixing [12]. Figure 17 illustrates the isocontours of the two parameters for a propagating triple flame. This parameterization highlights shifts in stoichiometry and reactions occurring in the three branches that may be obscured in physical coordinates when subjected to an unsteady vortical flow. Figure 18 shows the heat release and the fuel and oxidizer consumption rates presented in this phase space for the two instants $t/\tau_r = 0$ and 10. It clearly shows that, consistent with the description in physical coordinates, as the triple point is negatively strained, the peak heat release shifts to the lean limit, the peak consumption rates of the fuel and oxidizer are enhanced, and there is a more gradual transition between the premixed and diffusion flame branches. Figure 19 shows the corresponding radical reaction rates. Again, we observe that radical consumption disappears at the leading edge of the triple flame with straining, since defocusing of H coupled with the large curvature all but eliminates radical consumption at the tip. Instead, radical consumption is enhanced in the lean premixed and diffusion flame branches and radical production is enhanced due to focusing of hydrogen behind the flame tip.

CONCLUSIONS

Ignition and triple flame propagation were studied in a partially premixed hydrogen–air mixture with nonuniform mixing thickness using DNS with detailed chemistry. The main objective is to understand the structure and propagation characteristics of hydrogen–air triple flames compared to existing knowledge based on simple chemistry and other hydrocarbon systems.

For the diluted fuel stream case, for which the triple flame structure is nearly symmetric with respect to the stoichiometric line, the results from freely propagating triple flames suggest no substantial peculiar behavior compared to previous studies of methanol–air triple flames. The enhancement in the stabilization speed is
Fig. 18. Mixture fraction–temperature parameterization of triple flame for unstrained (a), (b), and (c) and strained (d), (e), and (f) cases. (a) and (d) denote heat release; (b) and (e) denote oxidizer consumption rate, and (c) and (f) denote fuel consumption rate.
Fig. 19. Mixture fraction–temperature parameterization of triple flame for unstrained (a), (b), and (c) and strained (d), (e), and (f) cases. (a) and (d) denote O atom reaction rate; (b) and (e) denote H atom reaction rate, and (c) and (f) denote OH reaction rate.
mainly due to flow divergence and additional flame-structure effect is very small, consistent with the results from the methanol–air system. We also found that, although the laminar flame speed of a homogeneous premixed flame is maximum for a rich mixture, for triple flames the heat release is shifted toward the lean side due to the prevalence of O₂, such that the triple point is bounded near the stoichiometric line.

For a mixing layer of undiluted hydrogen and air, the extreme asymmetric structure of the triple flames reveals some distinct features. One remarkable observation is that the maximum value of \( V_f \), and hence the actual stabilization point, occurs at a location different from the triple point at which heat release and the displacement speed are maximum.

The effect of flow strain on the triple flame behavior was also studied by imposing a pair of counterrotating vortices in front of the flame. As the triple point encounters compressive strain in the channel between the vortices, the premixed flame collapses onto the diffusion flame, thereby forming an edge flame structure. Subsequently, the shift in the heat release toward the lean premixed branch and the extinction of the H consumption layer at the tip were observed. The excessive compressive strain and curvature at the triple flame tip induced by the vortical flow results in negative displacement speed as observed in homogeneous turbulent premixed flames [19]. Finally, the \( \xi - T \) parameterization was shown to represent the structure of the triple flame with various flow strains in a systematic way.

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APPENDIX: VALIDATION OF NUMERICAL FIDELITY

While the computational expense for the two-dimensional simulation with complex chemistry makes it difficult to thoroughly test the effects of the initial ignition source and the domain boundary on the propagation speed, we have performed several one-dimensional problems to assess the effects indirectly. With a domain size
of $2.4L_r$, which is 1.5 times longer than the longitudinal domain length of the two-dimensional simulation, the stoichiometric premixed gas of hydrogen and air is ignited at the center of the domain. The Gaussian initial temperature profile as in Eq. 1 is imposed in the $x$-direction only, i.e.

$$T(x) = T_0 + (T_{\text{max}} - T_0) \exp\left[-\left(\frac{x - x_c}{\delta}\right)^2\right]$$ \hspace{1cm} (A1)

where $T_0 = 300$ K and $T_{\text{max}} = 3000$ K is used. Figure A1 shows the variation of the displacement speed, defined in Eq. 4, as the flame propagates from the center towards the end of the computational domain. It is demonstrated that, for $\delta = 0.05L_r$ that was used in the two-dimensional simulation, the displacement speed approaches the laminar flame speed within a few percent of error by the time the flame has propagated about $0.4L_r$, which is about halfway through the end of the longitudinal domain in the 2-D simulation. It is noted that the one-dimensional case is a more stringent test than the 2-D simulation, for which the initial temperature peak is expected to dissipate more quickly in the radial direction. As for the effect of the finite computational boundary, all three cases plotted in Fig. A1 show no sign of losing numerical accuracy until the flame front (defined as $Y_{H_2O} = 0.024$) reaches the end of the domain.

We have also performed an additional 2-D simulation in order to assess whether the flame-ball effect is important. In a reduced domain size of $L_x = L_y = 0.56L_r$, a mixing layer of a uniform thickness at $\delta = 0.05L_r$ is imposed in the horizontal direction and ignited at the $x = L_x$ boundary, such that only one triple flame is formed and propagates upstream. The fuel and oxidizer stream concentration is the same as the diluted case presented in this paper. An inflow velocity of $u = 2.09$ m/sec is also applied at the $x = 0$ boundary in order to maintain
sufficient distance between the triple flame and the inflow boundary throughout the simulation.

Figure A2 illustrates the evolution of the triple flame, represented by the $Y_{\text{H}_2\text{O}} = 0.03$ isocontour; Figure A3 shows the corresponding time history of $V_f$ and $S_d^*$ at the triple point for the data shown in Fig. A2. Both curves level off to a constant value after the triple flame is established. The asymptotic values are found to be $V_f/S_L^0 = 2.30$ and $S_d^*/S_L^0 = 0.96$, respectively. With the triple flame size comparable to the narrower triple flame in the original simulation, the value for $V_f$ is reasonably close to that shown in Fig. 9. Therefore, it is concluded that for a substantial duration of the simulation, say $t/t_r > 10$ shown in Figs. 9, 11, and 12, the reported values of the flame speed are indeed those of the freely propagating flames with negligible influence of the ignition source or the flame-ball effect.