Direct numerical simulation of premixed flame kernel-vortex
interactions in hydrogen-air mixtures

Short running title: Flame kernel vortex interactions

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Direct numerical simulation of premixed flame kernel-vortex interactions in hydrogen-air mixtures

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Abstract

The unsteady interaction between a vortex pair and a premixed flame kernel in 2D is investigated numerically using Direct Numerical Simulations (DNS) with a detailed reaction mechanism for hydrogen chemistry. The simulations are based on variations of the vortex size and strength with respect to a base case and in comparison with an unperturbed premixed flame kernel. The simulations result in two different regimes for flame kernel-vortex interactions, which based on the parameter range considered, are consistent with experimental observations. The first regime, the global extinction regime, is characterized by an interaction that is initiated when the kernel is still small compared to the vortex pair core size. The second regime corresponds to a later interaction in time when the kernel size is larger than the vortex pair core size, and resulting in primarily a wrinkling effect on the flame kernel. Computations of different global quantities show that the vortex-pair causes an enhancement in the flame surface area and the volumetric fuel consumption rate in the breakthrough regime. However, there is a reduction in the global consumption speed during the interaction associated with the effect of stretch on flame structure. A rescaling of the time scale, taking into consideration the vortex-pair translational velocity, is derived, which represents the main effect of the vortex-induced stretch on the flame surface area. Moreover, a new parameter is derived to evaluate the fraction of mutually interacting flames. Downstream interactions, which correspond to the proximity of flames from their burned gas side, are the dominant contribution to flame-flame interactions.
1. Introduction

Experimental and numerical modeling of the processes that govern combustion in turbulent flows presents several fundamental challenges. These challenges are a result of complex coupling, between chemistry, molecular and turbulent transport, over the entire range of length and time scales. In turbulent flames, the unsteady flow field continuously wrinkles the flame fronts, resulting in local extinction from straining, curvature and mutual flame annihilation by upstream and downstream interactions. The simple flame-vortex configuration can reproduce time-dependent effects of strain and curvature imposed on flame fronts. Many experimental and computational studies have been carried out in this area for a wide range of fuels, degrees of chemical complexity and burning models (premixed and diffusion) [1- 12].

A more recent extension of the laminar flame-vortex configuration is the flame kernel-vortex configuration [13]. In this configuration, a growing flame kernel issuing from an ignition source interacts with a toroidal vortex under conditions of varying mean curvature of the flame front. This configuration results in a progressive evolution of the range of eddy length scales that contribute to the wrinkling and the advection of the flame surface. Therefore, depending on the vortex strength relative to the flame speed and the flame kernel ‘maturity’ (the kernel size at the onset of interactions), different interactions regimes may be identified. Eichenberger and Roberts [13] investigated spark ignition of a lean methane mixture interacting with individual eddies of varying characteristic length and velocity scales. Spark-ignited kernel growth was observed in both the flamelet regime and the distributed reaction zone regime. Global quenching of the growing flame kernel was observed with sufficiently large vortices. Xiong and Roberts [14] studied the effects of laminar vortices of various sizes and strengths on a lean methane-air kernel under atmospheric conditions. Increases in the kernel growth rate by as much as a factor of three compared with an undisturbed kernel were observed. The maximum enhancement in the kernel growth rate was observed when the vortex interacted with a small flame kernel. Xiong and Roberts [15] studied the interaction between a lean-premixed spark-ignited flame kernel and a laminar toroidal vortex containing a different fuel/air mixture. They observed that vortices composed of fluids outside the traditional flammability limits were completely consumed by the kernel. The Lewis number of the vortex mixture determines if the vortex is consumed as a single pocket or breaks up into different pockets before being consumed. The experimental observations of Roberts and co-works [13-15]
illustrate the added complexity of flame kernel-vortex interactions relative to their planar counterparts.

Given the transient nature of the interactions and the inherent requirements to capture both flame dynamics and structure, important details about these interactions are not easily accessible via experiment. In the present work, we attempt to study numerically key aspects of flame kernel-vortex interactions associated with effects of these interactions on the flame structure and dynamics. The simulations are based on a simplified 2D geometry replacing the complex toroidal vortex by its equivalent in 2D, a vortex pair. Because of the important role played by chemistry during kernel-vortex interactions, the simulations are based on a detailed mechanism for a simple fuel, hydrogen. The effects of chemistry will be considered in more detail in future work to address processes of local and global flame’ extinction resulting from kernel-vortex interactions. The simulations, which are carried out at different vortex-pair characteristics, are used to study the effects of the vortex pair on the flame structure and kernel topology, and their implications to the global characteristics of the flame kernel: flame surface area and burning rate. In the following sections, the numerical implementation of the problem is presented (Sec. 2). Results are presented in terms of: 1) the important features of the three kernel-vortex interactions (Sec. 3), 2) the overall global characteristics of the flame kernel-vortex interactions (Section 4). Finally, conclusions of the key observations are presented in Sec. 5.

2. Numerical implementation

The computations are performed using Sandia’s S3D code in two dimensions [16]. The numerical scheme is based on the solution of the conservation equations for total energy, mass density, the two components of the flow velocity, and the mass densities of the components of the mixture in compressible flow. The governing equations are solved using an explicit eighth-order finite difference scheme for spatial derivatives [17] and a fourth order accurate Runge-Kutta scheme for temporal integration [18]. The boundary conditions, which are based on the NSCBC boundary conditions [19], and adopted to the present governing equations by Mahalingam [20], are non-reflecting in both the x and y directions. Temperature dependent properties are employed for the simulation using the formulation proposed by Smooke and Giovangigli [21] for the thermal conductivity, temperature dependent specific heats using the CHEMKIN thermodynamic database [22] and a Lewis number formulation for species mass transport Smooke and Giovangigli [21].
Lewis numbers are used to evaluate the species mass diffusivities, such that for a species identified with an index $k$, the Lewis number is expressed as $Le_k = \alpha / D_k$. Here, $\alpha$ is the thermal diffusivity, which may be expressed in terms of the kinematic viscosity and the Prandtl number as: $\alpha = \mu (\rho Pr)$. These Lewis numbers are evaluated by a least square fit of the species diffusive fluxes for a range of temperature between 500 and 2500 K using the premix code [23]. The Prandtl number is set at a constant value of 0.708. H$_2$ chemistry is based on the detailed H$_2$ mechanism of Yetter et al [24] with 9 species and 19 reversible elementary reactions. The values of the Lewis numbers for the different species used in the mechanism are given in Table 1.

The simulations are based on a 2 cm x 1.5 cm domain with a Cartesian grid of 1500 x 1125 grid points in the $x$ and $y$ directions, respectively. An Oseen [25] vortex model is used initialize the counter-rotating vortex pair. The tangential velocity profile contributed by each vortex, $u_\theta$, is given by,

$$u_\theta = \frac{\psi}{2\pi r} \left[ 1 - \exp \left( -\frac{r^2}{\sigma^2} \right) \right]$$

where $r = \sqrt{(x-x_0)^2 + (y-y_0)^2}$.

In this expression, $\sigma$ is the core radius of the vortex; the coordinates $(x_0, y_0)$ correspond to the center location of each vortex; and $\psi$ is the vortex strength, which may be expressed in terms of maximum tangential velocity, $u_{\theta,max}$, imposed at the radial location, $\sigma$ as follows:

$$\psi = \frac{2\pi}{1 - e^{-1} \times u_{\theta,max} \times \sigma} = 9.9399 \times u_{\theta,max} \times \sigma.$$  

Beyond the radial location of $\sigma$, the tangential velocity is set to zero. Four simulations are carried out. The first corresponds to an unperturbed (no vortex pair interactions) flame kernel. The remaining three simulations, referenced as cases A through C, correspond to a base reference case A, with a core radius of $\sigma = 0.1$ cm and a $u_{\theta,max} = 50$ m/s. The other cases B and C correspond to either variations in $\sigma$ or $u_{\theta,max}$. Case B corresponds to a ‘slower’ vortex, characterized by a factor of 5 reduction in $u_{\theta,max}$, and the same value of $\sigma$ relative to case A. Case C corresponds to a ‘larger’ vortex pair, characterized by a factor of 2 increase in the core radius, while $u_{\theta,max}$ is maintained the same as in case A. In all three cases, the values of $u_{\theta,max}$ are significantly higher than the reference laminar flame speed, $S_L$, favoring the role of the vortex pair on the dynamics of the flame kernel. The
different cases are summarized in Table 2. The distance between the vortex pair cores, although a potential separate parameter in the simulations, is set as the core radius, $\sigma$, for the different cases A through C. Another parameter, which corresponds to the distance between the vortex pair axis and the source of ignition, is set to the same value of 0.3 cm for all cases considered.

All cases, including A through C and the unperturbed kernel calculations, are based on the same mixture composition and ignition mechanism. A Gaussian temperature profile for the temperature is imposed initially. The profile has a peak value of 1800 K, and a characteristic thickness, which is equal to the laminar flame thickness, $\delta_F$. $\delta_F$ is the laminar flame thermal thickness expressed as $\delta_F = (T_b - T_u)/(dT/dx)_{\text{max}}$, where $T_u$ and $T_b$ are the unburnt and burnt gas temperatures. Figure 1 illustrates the configuration and indicates the various distance parameters chosen. As shown in Fig. 1 the vortices translate initially towards the ignition source (from left to right in Fig. 1).

A uniform and diluted H$_2$–air mixture is used in the current simulation such that the ratio by volume of H$_2$/O$_2$/N$_2$ is 1/0.5/5.13. The mixture is diluted in order to reduce the flame speed and affect a meaningful kernel–vortex interaction. The dilution leads to a reduced laminar flame speed, $S_L$, of 116 cm/s, based on the computed Lewis numbers and the DNS code in 1D. These Lewis numbers, listed in Table 1, are evaluated for this mixture composition. The effect of buoyancy is not considered in this study, and accordingly the gravity force is set to zero. The CPU time associated with the calculations of cases A through C and the unperturbed flame ranges between three to six weeks on 20 Intel Xeon 2.4 MHz processors. Although, some results presented here inherently could have been implemented with reduced chemistry, the present database is being constructed to also study details of local and global quenching in flame kernels.

3. Description of Important Features of Kernel-Vortex Interactions

In the following discussion, we illustrate the general features of the flame kernel topology subject to the different vortex conditions. The discussion identifies the different operating regimes found in the simulations and the mechanisms that affect the flame dynamics/topology and structure.

Figure 2 shows transient snapshots at increments of approximately 0.45 ms of the kernel vortex interaction corresponding to case A, visualized by contour plots of the heat release rate. The onset of interactions between the flame kernel and the vortex pair occurs at approximately 0.11 ms (a range that is not shown here). The kernel assumes a relatively flattened shape (at 0.11 ms), and then a
positively curved shape (at 0.145 ms) on the vortex pair’s side, and a negatively curved shape on the opposite side. Here, we denote positive curvature as curvature in which the center of curvature of the flame is on products’ side; while, negative curvature corresponds to a center of curvature that is on the reactants’ side (e.g. the flame tip of a Bunsen burner). The curvature of the flame is a result of the displacement by the vortex-pair induced velocity field of the flame surface. This displacement is strongest at the centerline and between the two vortices.

At 0.19 ms, the kernel begins to engulf the vortex pair, which shapes its contour; under unperturbed kernel growth, the kernel would assume a cylindrical shape. The process continues; and at 0.28 ms, the wrinkling effect of the vortex pair results in strongly curved flame tips between the flame sides that are propagating towards and away from the vortex pair. The kernel forms an envelope over the intruding vortex pair at 0.325 ms. Eventually, the vortex pair breaks through the leading edge of the flame kernel as shown at 0.45 ms. The process of kernel-vortex interactions exhibits important sub-processes that are outlined below:

- **Downstream Flame Interactions:** Downstream flame interactions correspond to interactions between flames starting from their products’ sides; and they are associated with the merger of at least one layer of the flame starting with the post-combustion zone. Further mergers of the reaction and preheat layers result in the local extinction of the interacting flames by mutual annihilation. During flame-kernel interactions, downstream flame interactions are most visible at the leading edge of the flame kernel as the vortex pair ‘forces’, through velocity gradients the trailing edge of the flame kernel into the leading edge, eventually reducing the distance of burned products between the two flames. The process is clearly shown at 0.415 ms as shown in Fig. 2.

- **Upstream Flame Interactions:** In contrast with downstream flame interactions, the process of upstream flame interactions is a result of the proximity of two flames from their reactants’ side. During this interaction, the two flames may be aided by their own propagation speed (towards each other) to accelerate their mutual annihilation. A number of conditions during kernel-vortex interactions can result in upstream flame interactions; but, they will be illustrated here along the narrow channel of nearly parallel flames on each side of the symmetry line formed by the straining of the flame at the wake of the vortex pair. This interaction is labeled in Fig. 2 at 0.37 ms. During the time window of the computations considered, the interaction is characterized by
the merger of the preheat layers; interactions between reactions layers would have followed at a later time.

- **Extinction by Strong Curvature:** This process is labeled at 0.45 ms. It results from the interaction of the two highly curved flame tips on each side of the horizontal symmetry line, resulting in the tips opening and extinction.

Figure 3 shows the transient snapshots of the kernel vortex interaction corresponding to case B, which involves a vortex pair of the same size but with a translational velocity 5 times lesser than case A. The interaction in case B is more prolonged and starts at a later time than the previous case. Snapshots are presented at time increments of 0.2 ms starting from 0.13 ms. The interaction begins with the flattening of the kernel on the vortex side at 0.13 ms and progresses in a qualitatively similar fashion to case A until 0.53 ms. The extinction at the flame tips attributed to curvature in case A (Fig. 2 at 0.28 ms) is not seen in case B for a similarly shaped kernel at 0.73 ms. This can be directly attributed to the lower translational and rotational attribute of the vortex in case B which induce lower curvature values on the kernel. At 0.93 ms opening of the flame tips is observed. This local extinction is caused by the downstream interaction of the flames defining the tip of the kernel.

A major qualitative difference between cases A and B is the extent and duration of the upstream interaction. In case A, due to the high rotational magnitude of the vortex pair, the flame segments which initially begin to interact at 0.37 ms are curved upwards delaying upstream interaction. In case B the flame segments curve into each other as shown at time 1.13 ms which leads to simultaneous upstream and downstream interactions unlike case A where the majority of the upstream interaction takes place after the downstream interaction at the leading edge. The vortex eventually “breaks-through” the kernel at approximately 1.53 ms.

Figure 4 shows the transient snapshots of the kernel vortex interaction in case C. The heat release rate magnitudes are at least one order of magnitude lower than cases A and B. The levels of the contours have been chosen to obtain the best visualization of the interaction. The vortex pair in this case has the same translational velocity as case A and twice the core radius, $\sigma$. Unlike the previous cases this interaction is characterized by the global quenching of the kernel. The transient snapshots are at an interval of 0.01 ms starting from 0.12 ms. The kernel comes into the region of influence of the vortex pair at 0.12 ms. The size of the kernel is appreciably smaller than cases A and B which indicates that the enlarged vortex pair affects the growth of the kernel from an early time. The kernel
assumes a flat shape on the vortex side at 0.13 ms. Local extinction is seen at the flame tips at 0.14 ms with further flattening and elongation of the kernel. A reduction in the heat release rate at the core of the flame kernel is observed at 0.15 ms. The kernel then progressively evolves towards global extinction.

In the above discussion, two distinct regimes have been illustrated. The first is the ‘break-through’ regime corresponding to cases A and B. In this regime the kernel is able to evolve around the smaller vortices and engulf them. The interaction eventually leads to the vortex pair ‘punching’ through the leading edge of the kernel. The second is the ‘extinction’ regime. In this regime, the evolution of the kernel and its growth is radically affected by the vortex pair. The kernel cannot sustain the imposed high strain rates by the imposed vortex-induced velocity fields and is globally extinguished. While the two cases, A and B, which correspond to the break-through regime, are qualitatively similar, and the flame topologies exhibit different details in different flame sections.

An important distinction between operations at the two regimes can be pointed out based on the cases simulated. Global extinction is associated with the larger (i.e. compared to the kernel size) scale motion induced by the vortex pair. This large scale motion sustains high strain rates on the entire flame surface. In the break-through regimes, the kernel mean radius evolves to a stage where it is larger than the vortex pair; therefore, the vortices contribute to the wrinkling of the flame surface with the extent of straining and other interactions are imposed locally at different rates and at different sections of the flame. The two effects ‘global straining’ vs. wrinkling represent the contribution of large scale and small scale vortices in turbulent flame kernels, respectively. Additional contributions to the evolution of the flame surface have already been pointed out, including flame annihilation by upstream and downstream interactions.

Though a difference exists in the nature of the fuels and the time scale of the interactions studied experimentally by Roberts and co-workers [13-15] and computationally here, the simulation results are consistent with the key observations in [13-15]. Qualitatively the profiles of the flame surface in Xiong and Roberts [14] show some features of the computational simulations. The kernel is flattened on the vortex side as in the present study. Though the vortex does not break through the leading edge the kernel it does however significantly distort the kernel. The wake of the vortex is similar to the flame envelope undergoing upstream interaction in case B. In [14] the vortex does enhance the growth of kernel which corresponds to the increase in the flame area shown in the present study. In
the same study, an increase in the integrated chemiluminescence intensity is observed, which is verified by the increase in the integrated volumetric reaction rates in the present computations. In [14] the unperturbed kernel shows a linear growth in the kernel radius. In the simulations the kernel flame area which is a linear function of the kernel radius for an unperturbed kernel shows two distinct slopes. As mentioned previously this effect is because of the lingering excess heat of ignition which hastens kernel growth initially. Also global extinction of the flame kernel experimentally has largely been observed for large a vortex [13] which is one of the conclusions of the present study.

4. Evolution of Global Measures of Flame Surface Area and Structure

The kernel-vortex interactions result in important straining of the flame surface; and therefore they contribute to its growth relative to an unburned kernel. At the same time, other effects contribute to important changes to the flame structure as a result in flame-flame interactions or the evolution of flame topology (strain and curvature). We will try to assess the result of the competition between flame surface area growth and local changes in flame structure, and the effect of this competition on volumetric rate quantities, such as the fuel consumption rate. The comparisons will be made among the different cases, in particular with respect to case A, and also with the unperturbed flame kernel. It is important to note here that while we may refer to the customary concepts of flame surface area and volumetric consumption rates, our 2D results actually generate flame surface areas and area-integrated consumption rates. In the present work, we will adopt the 3D nomenclature, and present results based on our 2D calculations and per unit depth in the third direction.

4.1. Evolution of the Flame Surface Area

To evaluate the flame surface area at different times of the computation, we track the evolution of a contour of a fixed progress variable (a normalized temperature), \((T-T_u)/(T_b-T_u)\), with a value of 0.6. Figure 5 shows the temporal evolution of the flame surface area for the cases A through C and the unperturbed kernel. Initially, the flame surface area is zero, and after an ignition delay time of approximately 0.05 ms, the area starts to increase. All cases show a similar rapid initial increase in the flame area. This increase is partly due to flame propagation away from the ignition source, but mostly to the expansion of the products of combustion. Both mechanisms are present in both perturbed and unperturbed flame kernels.

The flame area growth for the unperturbed kernel exhibits two global trends in time: one immediately after ignition, and the other at a later time. The first trend corresponds to the rapid
expansion of hot products, which carries with it the propagating flame kernel. The process of expansion, although inherent in premixed flame propagation, is enhanced by the confinement of hot products, which expand outwardly away from the ignition source. The initial rate of gas expansion is as much as one order of magnitude higher than the laminar flame speed. As the kernel size grows, the effect of this rapid expansion process is decreased; and the rate of flame surface area increase approaches a constant slope.

Cases A and B exhibit higher flame areas in comparison with the unperturbed kernel; but, the rates of the flame surface area growth for the two cases are different, with the ‘faster’ vortex case, case A, exhibiting the higher value at a given physical time. The different behavior in the rate of kernel growth for the two cases when compared to the unperturbed kernel can be directly attributed to stretch effects on the flame induced by the vortex pair. Without this stretch, the only mechanisms responsible for flame surface area growth are flame propagation and the expansion of burned gases. The evolution of the flame area for case B shows two differing slopes before and after 0.8 ms, which corresponds approximately to the time when the kernel starts to engulf the vortex pair. The flame surface length for case C increases initially and at a rate slightly faster than that of the unperturbed flame kernel. However, as global extinction is initiated, the flame surface area reaches a peak at approximately 0.14 ms, and then decays to zero at approximately 0.18 ms.

From Figs. 2-3 and the discussion above, the dominant mechanisms, which contribute to flame kernel surface growth or reduction may be identified as follows: 1) flame stretch and 2) flame extinction. Within each contribution, other contributions can also be identified. For flame stretch, the ‘kernel-induced stretch’, which is inherent in the unperturbed flame kernel, is a result of the formation of a kernel from an ignition source and the resulting expansion of this kernel by virtue of its propagation and the burned products’ expansion. As stated, the contribution from this mechanism can be evaluated using the unperturbed kernel. The second mechanism associated with stretch is the ‘vortex-induced stretch’. From the figures, it is evident that a major contribution of this stretch occurs in the streamwise direction, resulting in an elongated flame kernel in that direction.

The mechanisms associated with extinction can be related to either global extinction, as observed in case C, or local extinction as seen during the evolutions of cases A and B. In both conditions, the principal mechanisms can be associated with ‘hydrodynamic stretch’, including the effects of curvature in case A and B, and curvature and strain in case C, and flame-flame interactions. In case
C, both hydrodynamic stretch effects and flame-flame interactions are present during the global extinction process. Both effects interrupt the combustion process on the products’ side of the flame; and therefore, their contribution can not be dissociated. In the following discussion, we address two key mechanisms, which contributed to flame kernel surface growth or reduction: ‘vortex-induced stretch’ and flame-flame interactions.

4.2. Contributions to flame surface area growth: vortex-induced stretch

The magnitude of stretch imposed on the kernel by the vortex determines the transient behavior of the flame area curves relative to the unperturbed flame kernel. The resulting outcomes are different slopes for the temporal evolution of the flame kernel surface area based on the imposed vortex conditions. In Fig. 5, it is evident that while vortex core size contributes to whether a kernel undergoes global extinction or break-through (comparison between case A and C), different vortex translation speeds contribute to the rate of flame surface area growth (comparison between cases A and B). Therefore, based on the conditions considered, the vortex-pair translational speed plays a key role in flame stretch. In what follows, a simple model is proposed, which accounts for the dominant contribution represented by vortex-induced flame stretch in the break-through regime.

A principal assumption is used here, and is being deduced from Figs. 2 and 3: in comparison with the unperturbed flame, a key additional contribution to the flame area is represented by the inner flame channel produced at the trailing edge of the vortex pair. The rate of growth of this channel is assumed to be proportional to the vortex-pair translational or displacement velocity, \( V_d \). This velocity is of the same order of \( u_{\theta,\text{max}} \); but, it is primarily determined by the distance between the cores of the vortices, and the vortices’ temporal evolution due to vortex-vortex interactions, viscous dissipation and heat release. The perturbed flame kernel area, \( A \), for both cases A and B is expressed as a function of the unperturbed kernel area, \( A_u \), and the translational velocity, \( V_d \), as follows

\[
A = A_u + \alpha V_d t,
\]

where \( \alpha \) is a proportionality constant. A simple analysis of the contribution of the growth of the flame channel made up of two flames opposite the symmetry line suggests that the value of \( \alpha \) is approximately 2. However, the present data suggests a lower value of approximately 1.3 based on an averaged vortex displacement speed. A non-dimensional time, \( t^* \), and a non-dimensional flame surface growth relative to the unperturbed flame, \( A^* \), can be expressed as:

\[
t^* = \frac{(\alpha V_d t)}{\delta_p}
\]

and
$A^* \equiv (A - A_s)/\delta_F$, respectively. We also take the value of $V_d$ to be a time-averaged translational speed of the vortex pair during the interactions’ time considered. Figure 6 shows the variation of $A^*$ vs. $t^*$. In the time range considered, which corresponds to the extent of the unperturbed flame simulation (0.64 ms), the average translational velocities, $V_d$, for cases A and B are 34.8 m/s and 8.5 m/s, respectively. Therefore, in comparison with the values of $u_{\theta,\text{max}}$, the values of $V_d$ are lower than $u_{\theta,\text{max}}$; and they are for cases A and B approximately 0.7 $u_{\theta,\text{max}}$ and 0.85 $u_{\theta,\text{max}}$, respectively. Figure 6 shows that the proposed correlation does not collapse exactly the modified flame areas for cases A and B. However, the two profiles are very close, especially at later reduced times in the interactions, where they are within less than 15% of each other. The difference can be contrasted with the flame area evolution profiles given in Fig. 5. Moreover, the two flame area profiles exhibit similar slopes away from the ignition time suggesting that the scaling of $A^*$ with $t^*$ is reasonable for the range of physical times considered, and accounts for the bulk of the contribution from the vortex-induced stretch.

4.3. Contributions to flame surface area growth: flame–flame interactions

As indicated earlier, important flame-flame interactions are present during the flame kernel-vortex interactions. These interactions result in important effects on the volumetric heat release rate and the flame surface area. In this section, we attempt to illustrate the mechanisms by which flame-flame interactions contribute to the rate of flame surface growth and heat release.

The degree by which flame-flame interactions contribute to flame shortening is measured through a new parameter that is introduced here: the flame interactions’ fraction, $I$. The parameter, $I$, is expressed as the fraction of the flame surface that is within close proximity to another flame along its normal. This distance is assigned to be of the order of half the thermal flame thickness; and other fractions of the flame thickness between 0.25 and 0.5 yield essentially the same trends in the magnitude and shape of the temporal profiles of $I$. The fraction, $I$, is evaluated numerically by the following procedure:

- First, a flame isocontour is evaluated based on the same procedure adopted for the evaluation of the flame area.
- This isocontour is divided into small incremental segments that span this isocontour.
• On each segment, a box delimited by this segment, and extending normal to it. The extent of this box (i.e. its thickness) is a fraction of the flame thickness; and it is 0.5 $\delta_F$ in this case.

• Within this box, a search for segments from neighboring isocontours (i.e. flames) is carried out; and the total length within each segment is computed. When summed over the entire flame isocontour, and the sum is divided by the total length is the isocontour, the resulting fraction is the flame interaction fraction, $I$.

In this study, we further distinguish between the fractions of flames undergoing upstream interactions, $I_u$, from those undergoing downstream interactions, $I_d$. This distinction is based on the direction from the flame segments in which the box along the normal is defined. If this direction is towards (resp. away from) the products, the parameter corresponds to a downstream (resp. upstream) interaction. Therefore, the direction for the search along the flame normal is carried out either in a direction of increasing value for the progress variable to track downstream interactions, or in the opposite direction to track upstream interactions.

Figure 7 shows the percentage fraction of the flame undergoing downstream mutual interaction. Case A shows the highest percent fraction of flame surface area undergoing downstream interaction. It is apparent that cases A and B have a similar temporal evolution of the fraction of the flame area undergoing downstream interaction. A first interaction occurs when the kernel is still small compared to the vortex pair. As indicated in Figs. 2-3, at this stage the kernels assume a relatively flat shape with two strong highly curved tips. It is at these flames tips that the initial downstream interactions occur; and in principle cannot be dissociated with the role of curvature. At a later stage, downstream interactions are governed by the proximity of the leading and trailing edges of the flame. At this stage, the initial kernel expansion pushed these two edges apart; but, as this expansion is reduced in time, the vortex pair pushes the trailing edge closer to the leading edges. The two flame edges approach each other from their burned gas sides. The second stage of downstream interactions results in a higher fraction of flames undergoing downstream interactions. In Fig. 3 corresponding to case B, this process results in a significant reduction in the heat release rate at these flame edges. The onset of this stage of downstream interaction for the two cases occurs past 0.34 ms for case A and past 1 ms for case B. Moreover, this interaction at the leading edge is extremely rapid in case A and takes place from approximately 0.34 ms to 0.4 ms; while, the corresponding rate for case B is
significantly shorter. The time scale of the interaction at the leading edge is dictated by velocity gradient imposed by the vortex pair at the leading edge.

In case C, the initial stage of the downstream interactions results in a higher fraction, $I_{d_s}$, during the ignition phase reaches a maximum value 6% of the flame kernel experiences downstream interaction, a value significantly lower than the corresponding values in kernels A and B. The fraction, $I_{d_s}$, eventually decays to zero after the kernel is completely extinguished. Therefore, downstream interactions in kernel C are sustained during the lifetime of the kernel.

Figure 8 shows the percent fraction, $I_u$, of the flame kernel undergoing upstream interactions for kernels A and B. In case C, this fraction is identically zero; and therefore, it is not shown here. By comparing the percentage fractions of upstream and downstream interactions at the flame kernel, the overall magnitude of $I_u$ for cases A and B is lower than $I_d$ for the same cases; a smaller fraction of the flame kernel is subject to downstream interactions compared to upstream interactions. It is evident that downstream interaction plays a dominant role for cases A and B, at least during the break-through stages.

The principal contribution to upstream interactions in case B results from the presence of the flame ‘channel’ trailing the vortex pair. The rate at which this channel closes is governed by flame propagation, a much slower process than the downstream interaction process seen at the kernel’s leading and trailing edges. A longer simulation time for case A would have shown an increasing fraction, $I_u$ corresponding to the closing of the trailing flame channel; and the bulk of contribution to $I_u$ comes from the leading edge of this channel as delimited by the box in Fig. 2 corresponding to 0.37 ms.

4.4. Volumetric consumption rates of $H_2$

Equally important global quantities, in addition to the flame surface area, are volumetric rates corresponding to reactants’ consumption, products’ formation or heat release. In this section, we study the evolution of the volumetric consumption rate for the fuel, $H_2$. This rate is computed by (area) integration over the computational domain of the rate of fuel consumption: $\int A \int \omega_{H_2} dxdy$, where $\omega_{H_2}$ is the rate of fuel consumption (in g/cm$^3$-s). As implemented for the flame area, the volumetric fuel consumption rate is based on a 1 unit depth. Since the growth of flame surface area is an important contribution to volumetric fuel consumption rate, we will attempt to identify the extent of
this contribution, and in a later section evaluate the contribution resulting from changes to the burning intensity of the flame kernel as a function of time.

Figure 9 compares the temporal evolution of the volumetric reaction rates of H$_2$ consumption for cases A through C and the unperturbed kernel. The volumetric reaction rate for case C is similar to the behavior of its flame area. It peaks at approximately 0.14 ms; and then decays due to the kernel’s global extinction; but, the departure from the unperturbed kernel rates occur earlier than that of the flame surface area. The trends of the volumetric reaction rates of H$_2$ for cases A and B are initially similar to those of the unperturbed kernel; and they are characterized by a rapid increase over the first 0.2 ms. Beyond this time, the slopes for the different cases are lower. Again, the volumetric H$_2$ consumption rates also exhibit consistent trends to those of the flame surface area for cases A and B and the unperturbed kernel. However, the corresponding magnitude ratio is lower than that of the flame area. The relative magnitudes of the volumetric H$_2$ consumption rates between case A and B can be partially attributed to the differences in the flame areas between the two cases. Other factors are discussed in detail below, and are associated with the competing effects of stretch on the local flame structure. Therefore, for the two cases A and B an increase in the flame area does not reproduce a proportional increase in the volumetric reaction rate. Therefore, the effects of kernel-vortex interactions on the flame structure counter those associated with the kernel area growth, resulting in similar temporal profiles for the volumetric fuel consumption rates for cases A, B and the unperturbed kernel.

4.5. Evolution of the volume-averaged consumption speed

The net effect of kernel-vortex interactions on the flame structure can be illustrated by evaluation of a volume-averaged consumption speed, $\langle S_{c} \rangle_{vol}$, which is expressed as the ratio of the volumetric consumption rate of H$_2$ and the flame surface area:

$$\langle S_{c} \rangle_{vol} = \frac{\int \dot{\omega} \, dx \, dy}{A_{Flame} \rho_{u} (Y_{F,b} - Y_{F,u})}.$$  \hspace{1cm} (5)

In this expression $Y_{F,b}$ and $Y_{F,u}$ are the fuel mass fractions at the burned and unburned gas, respectively; $A_{Flame}$ is the flame surface area (or length) (see Fig. 5). $\langle S_{c} \rangle_{vol}$ may be normalized by the steady planar laminar flame speed, $S_{L}$, which also corresponds to the consumption speed for this reference flame. A ratio greater than unity indicates an enhanced rate of burning resulting from
flame-flame and flame-flow interactions; while, a ratio lower than unity indicates a reduced rate of burning resulting from these interactions.

Figure 10 shows the temporal evolution of this ratio for H₂. The figure shows that the flame kernel profiles, with and without the vortex pair, initially start with a higher rate of fuel consumption than the steady planar flame. The high values of $\langle S_{c} \rangle_{\text{vol}}$ can be attributed to preheating effects, which are responsible for the ignition process. Variations of up to 10% during this period can be seen in the magnitude of $\langle S_{c} \rangle_{\text{vol}}$ due to the choice of the location of the progress variable isocontour within the reaction zone used to track the flame surface. The choice of the isocontour is less important at later times, as the kernels’ radii grow significantly larger than the flame thickness. At a later time, the normalized $\langle S_{c} \rangle_{\text{vol}}$ value in the absence of a vortex pair approaches unity. This is expected as the kernel evolves away from the ignition source and assumes a more planar flame shape.

On the other hand, the normalized value of $\langle S_{c} \rangle_{\text{vol}}$ in the presence of a vortex pair decays at a much faster rate. In case C, $\langle S_{c} \rangle_{\text{vol}}$ decays to zero, signaling the onset of global extinction, at the same time the volumetric H₂ consumption rate too is reduced to zero. In cases A and B, the values of $\langle S_{c} \rangle_{\text{vol}}$ also decay relatively fast initially; then, this decay is slower at later interactions. For the length of the simulation case B also approaches a nearly asymptotic value that is below 40% the steady laminar flame value, $S_{L}$. Case A exhibits a similar trend, and approaches a lower value below 30% the steady laminar flame speed, $S_{L}$. Different competing factors may contribute to the trend of $\langle S_{c} \rangle_{\text{vol}}$ at the later times of the simulations. First, flame sections undergoing local extinction eventually evolve into extinguished kernels with no contribution to the flame surface; this trend tends to increase the $\langle S_{c} \rangle_{\text{vol}}$ once the flame section is extinguished. Meanwhile, other sections of the flame continue to undergo important reduction to their burning intensity. Therefore, the process observed, as indicated by the leveling of $\langle S_{c} \rangle_{\text{vol}}$ in time, may be temporary; and other trends for $\langle S_{c} \rangle_{\text{vol}}$ at later times of the interactions past the break-through stage may be found.

5. Conclusions

The kernel vortex interaction for a diluted H₂-air mixture has been studied. The impinging vortex causes significant distortion of the kernel topography. Various facets of turbulent premixed
Combustion-like flame-flame interactions, curvature and strain effects and local extinction are observed. These include global and local extinction involving both effects of hydrodynamic stretch and flame-flame interactions. Also, the vortex pair plays different roles depending upon the size relative to the flame kernel. In turbulent flames, these roles represent the contribution of the different scales of turbulence to flame structure and dynamics.

Two distinct regimes are simulated in the present study: a “break through” where the vortex pair ‘punches’ through the kernel, and a global extinction regime where the vortex pair completely quenches the kernel. The vortex pair causes an enhancement in the flame kernel growth and the volumetric reaction rate in the “break through” regime. This enhancement is identified as a vortex-induced stretch. A simple normalization in time based on the vortex pair translational speed results in similar area enhancement profiles relative to an unperturbed kernel. The increased flame surface area relative to the unperturbed flame for kernels in the break through regimes is reflected in the higher rates of volumetric fuel consumption (and accordingly heat release). These higher rates, however, are tempered by the presence of extinction due to vortex-induced stretch and flame-flame interactions. The normalized volume-averaged consumption speeds for the three cases are lower than the 1-D laminar flame values. The lower values signify an overall reduction in the burning intensity of the kernel. The extent of upstream mutual annihilation depends on the translational velocity of the vortex. The new parameters, $I_u$ and $I_d$, which measure the fraction of flames subject to flame-flame interactions will be explored in the future to address modeling strategies for the flame surface and the flame surface density function in flamelet-based models; and their value extend beyond their application here to flame kernels.
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<tr>
<td>H₂  O₂  O OH H₂O H HO₂ H₂O₂ N₂</td>
</tr>
<tr>
<td>0.31 1.14 0.74 0.75 0.86 0.19 1.14 1.15 1.29</td>
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</tbody>
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<table>
<thead>
<tr>
<th>Case</th>
<th>Maximum radial velocity in each vortex, $u_{\theta,max}$ (m/s)</th>
<th>Core radius of each vortex, $\sigma$ (cm)</th>
<th>$u_{\theta,max}/S_L$</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>50.0</td>
<td>0.1</td>
<td>43.1</td>
</tr>
<tr>
<td>B</td>
<td>10.0</td>
<td>0.1</td>
<td>8.6</td>
</tr>
<tr>
<td>C</td>
<td>50.0</td>
<td>0.2</td>
<td>43.1</td>
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Figure 3. Transient snapshots of heat release rates for Case B. The heat release rate is normalized to yield non-dimensional quantities. The domain size is 2 cm in the direction of vortex propagation and 1.5 cm along the second axis.

Figure 4. Transient snapshots of heat release rates for Case C. The figure also shows superimposed vorticity (white lines) with counterclockwise vorticity in solid lines and clockwise vorticity in dashed lines. The heat release rate is normalized to yield non-dimensional quantities. Note the range difference between case C and cases A and B. The domain size is 2 cm in the direction of vortex propagation and 1.5 cm along the second axis.

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