Extinction of stratified counterflow $H_2/air$ premixed flames under intense turbulence and strain

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Highly turbulent lean premixed hydrogen-air flames stabilized against counter-flowing non-adiabatic stoichiometric combustion products in chemical equilibrium are investigated in a joint numerical and experimental effort. The effects of turbulence, strain rate, non-adiabaticity and composition stratification on flame structure, local flame quenching and re-ignition are studied using three-dimensional Direct Numerical Simulations (DNS) and laser induced fluorescence (LIF) imaging of OH. Combustion was established at an elevated turbulent Reynolds number of 1,500 and a bulk strain rate of 2400 s$^{-1}$ in a compact cylindrical volume delimited by the two co-axial nozzles of diameter 12.7 mm and separation distance of 12 mm. The reactant and equilibrium product streams are at temperatures of 294K and 1475K respectively, and at 1 atm. Computationally, the compressible Navier-Stokes, total energy and species conservation equations are solved using a high order, low-dissipative finite difference scheme. An explicit Runge-Kutta scheme is used for time integration. A detailed chemical kinetics mechanism for hydrogen-air combustion is used, that involves 9 species and 19 elementary reaction steps. The code is parallelized with MPI message passing routines. The analysis of the combined numerical and experimental data aims to quantify the local extinction levels and examine the morphology of the extinguishing and re-light events. The joint approach focuses on a detailed presentation of the turbulence-flame interactions and an assessment of the driving mechanism that leads to the appearance of non-reactive regions along with the main re-ignition patterns. The main objective is to provide a combined numerical and experimental database and achieve in-depth physical understanding of the fundamental and complex mechanisms associated with local extinction and flame healing in turbulent stratified combustion.

1. Introduction

The design of efficient, low emissions internal combustion engines operating on alternative fuels unaffected by safety concerns is the subject of extensive research both at the industrial and academic levels. State-of-the-art combustors operate under intense turbulence and strain and often achieve flame stabilization by mixing of reactants with hot combustion products. These design strategies have a strong impact on the combustion processes and ultimately influence the fuel consumption rate and the pollutant formation. Increased turbulence intensity and strain rate can be desirable as they enhance mixing; however, they can simultaneously lead to operability issues such as flame blow-off, flashback and thermo-acoustic instabilities. Flame stability can be strengthened by the heat supplied from combustion products, however, dilution and radical depletion of the reaction zone in stratified regions may lead to weakened unstable flames and partial extinction.

Experimental investigation of finite-rate chemistry effects in turbulent premixed flames is a challenge. The requisite combination of high turbulence intensities and weak burning rates are required that may inevitably lead to full quenching of the flame. For instance, the blowoff of
premixed flames in turbulent counterflowing jets of fresh reactants is well understood (Kostiuk et al., 1993; Coppola et al., 2009). In this configuration increased flow rates or reduced nozzle distance increases the bulk strain rate, while adding diluents or reducing the equivalence ratio of the reactants reduces the burning intensity. Both effects force the twin turbulent flames to merge and annihilate each other. Pilotled flames, intense swirl and bluff-bodies designed for local mixing of the reactants with hot combustion products have been used to stabilize turbulent premixed flames at elevated Karlovitz numbers (e.g., Mansour et al., 1998; Dunn et al., 2010; Cabra et al., 2005); however, the mixing of the reactants and pilot gases is disregarded in turbulent premixed combustion regime diagrams (e.g., Peters, 2000).

Numerical studies of finite-rate chemistry effects in turbulent premixed flames faces two challenges from a computational feasibility perspective: full consideration of finite-rate chemistry effects requires a large number of transported chemical species, and premixed flames typically involve very fine spatio-temporal chemical scales that require a high degree of spatial and temporal resolution. However, with available computational power continually increasing, well resolved Direct Numerical Simulations (DNS) of turbulent combustion – hitherto confined to small computational domains and modest Reynolds numbers – has begun to approach laboratory scale configurations (Yoo et al., 2009; Grout et al., 2012). It is now feasible to simulate the physical extent of compact high Reynolds number laboratory scale configurations for short periods of time, i.e. long enough to capture and temporally resolve intermittent flame/flow dynamics, but not long enough to attain converged statistics. DNS provides complementary information by informing experiments of the importance of three-dimensional turbulence and flame structure and by temporally and spatially resolving intermittent events which may not be resolved even by high-speed imaging.

In the present study, a counterflow turbulent burner is employed in the study of localized extinction and reignition dynamics in turbulent premixed $H_2/\text{air}$ flames. The counterflow configuration, depicted in Fig. 1, consists of a jet of fresh premixed reactants opposed against a second jet of combustion products in thermochemical equilibrium. Under certain conditions, a single turbulent premixed flame is stabilized against the counterflowing stream of sub-adiabatic combustion products. The interaction of the premixed flame front with the counterflowing products can lead to localized extinction and, therefore, non-flamelet behavior (Coriton et al., 2011). However, the mixing of fresh reactants with the counterflowing products can eventually lead to localized auto-ignition, for a certain range of thermochemical and flow conditions. Recently, Coriton et al., 2013 used this counterflow system to systematically study the effects of heat loss, reactant stoichiometry, bulk strain rate and turbulence on localized extinction and ignition in premixed methane-air flames.

In the present contribution, we investigate the dynamics of partial quenching and re-ignition in a joint experimental and numerical approach. The purpose is to complement the characterization of these processes from past experiments with a more in-depth understanding that can be gained using DNS. In the experiments, laser-induced fluorescence (LIF) is used to characterize the flame structure and identify localized extinction in the $H_2/\text{air}$ as in the $CH_4/O_2/N_2$ premixed flames previously studied.

The paper is structured as follows. A brief description of the experimental setup is provided in the next section. Section 3 provides an outline of the numerical simulations performed. Results are presented and discussed in Section 4 and conclusions are summarized in the final section.
Figure 1: Schematic of a turbulent counterflow flame. The OH-LIF signal was analyzed in the 10 x 10 mm² red dashed square box and the DNS data in a 6.6 x 8 x 8 mm³ rectangular volume denoted by the blue dotted box in the xy-plane of the schematic. The full DNS domain includes the co-flow and is 12x17.5x17.5 mm³.

2. Burner design and experimental configuration

The design of the counterflow system has been detailed in previous work (Coriton et al., 2011; Coriton et al., 2013). Briefly, the burner consists of two axisymmetric, opposed nozzles of internal diameter $D = 12.7$ mm and separated by a distance, $L_x = 12.0$ mm. The flow arrangement consists of a turbulent stream of premixed reactants supplied through the upper nozzle at a volume flow rate of $Q_u = 110$ LPM and at an inlet temperature of $T_u = 294K$ and a laminar stream of hot combustion products supplied through the bottom nozzle at $T_b = 1475K$. The reactant stream is shielded from the ambient air by an annular co-flow of nitrogen, supplied at 85 LPM. Anisotropic turbulence is generated using a turbulent generator plate (TGP), (Coppola et al., 2009), and was fully developed within the upper nozzle. The upper-jet turbulent Reynolds number $Re_t = 1,435$ is defined as $Re_t = v'_o l'_o / \nu_{N_2}$, where $\nu_{N_2}$ is the nitrogen kinematic viscosity at 294K, $v'_o = 5.15m/s$ is the Root-Mean Squared (RMS) velocity fluctuation, and $l'_o = 4.2 mm$ is the integral length scale. The parameters $v'_o$ and $l'_o$ are measured on the nozzle centerline at 0.5 mm downstream of the nozzle exit using hot-wire anemometry (HWA) in a turbulent free-jet of nitrogen delivered through the upper nozzle (Coppola et al., 2009; Coriton et al., 2013). The reactant composition was a mixture of hydrogen and air with an equivalence ratio of $\phi_u = 0.4$. The freely-propagating laminar flame speed and thermal flame thickness computed using the DNS solver S3D, is detailed in the next section, were $S_L = 0.22 \text{ m/s}$ and $l_f = 0.14 \text{ mm}$, respectively. As a result, the turbulent burning conditions correspond to a turbulent Karlovitz number $Ka_t = (v'_o / S_L)^{3/2} / (l'_o / l_f)^{1/2}$ of 21. The bottom stream of hot combustion products is delivered by a stoichiometric $H_2/air$ premixed flame enclosed inside the nozzle ($Q_b = 85$ LPM, measured at 294 K).

The OH-LIF measurements are performed in a plane intersecting the burner centerline. OH-LIF is excited at 283.01 nm to pump the $Q_1(6)$ transition of the $A-X(1,0)$ band of OH. An intensified
A CCD camera with a f/1.8 quartz camera lens is used to record the OH-LIF signal with a spatial resolution of 50 μm × 50 μm. The image intensifier is gated for 500 ns bracketing the dye laser pulse. The OH-LIF images are corrected for spatial variations in the laser sheet using OH-LIF measurements in the product region of a burner-stabilized flat premixed flame to record the beam profile. The combination of a UG11 color glass filter and a high-transmission bandpass filter (Tr. > 80%, λ = 305-325 nm) transmitted the OH fluorescence from the (0,0) and (1,1) bands and blocked out-of-band interferences. The OH-LIF images are also corrected for variations in laser energy along the direction of beam propagation that resulted from absorption. The OH LIF images are cropped to the region of interest indicated in Fig. 1.

3. Numerical Simulations

Direct Numerical Simulation is employed to computationally investigate the structure and evolution of highly turbulent H2/air counterflow flames. The configuration is well-suited for computational studies of turbulent flames as the flames stabilize in a compact cylindrical volume and away from solid boundaries. The compressible Navier Stokes, species continuity and total energy equations are solved on a Cartesian three-dimensional structured grid using a massively parallel DNS solver, S3D (Chen et al., 2009). A fourth-order, six-stage, explicit Runge-Kutta scheme is used for time integration, (Kennedy et al., 2000), and an eighth-order central spatial differencing scheme is used to approximate the spatial derivatives along with a tenth-order filter to remove any spurious high frequency fluctuations in the solution, (Kennedy et al., 1994). A detailed H2/air kinetic mechanism (Li et al., 2004) is used to describe hydrogen oxidation consisting of 9 species and 21 chemical reactions. Reaction rates, thermodynamic and mixture averaged transport coefficients are evaluated using the CHEMKIN and TRANSPORT libraries, (Kee et al., 1996a; Kee et al., 1996b) which are linked with S3D. Navier-Stokes characteristic boundary condition (NSCBC) treatment (Yoo and Im, 2007) is imposed at the physical boundaries which are nonreflecting inflow in the streamwise direction (x = 0 mm and x = Lx) and non-reflecting outflow at all lateral boundaries (y = 0 mm, y = Ly, z = 0 mm, z = Lz).

The three-dimensional computational domain consists of 432 × 640 × 640 grids in the x, y and z directions, respectively and extends 0.95D × 1.48D × 1.48D. An equidistant Cartesian grid is used in all three directions, where the resolution is carefully chosen to adequately resolve both the flame and turbulent flow field, resulting in a uniform spacing equal to Δx = 470. The required flame resolution is identified from one-dimensional tests performed at different resolutions and ensures that all radical profiles and reaction rates are sufficiently resolved. The composition of the sub-adiabatic product stream is obtained from an equilibrium calculation of a stoichiometric H2/air flame performed using EQUIL (Reynolds, 1986). The reactant and product stream discharge bulk velocities \( U^r_j \) and \( U^p_j \) are obtained from the experimental volume flow rates of the two jets. The mean jet velocity profile at the nozzle exit is curve-fitted using a hyperbolic tangent function.

To reproduce the turbulence generated by the turbulence generator, velocity fluctuations are superimposed on the mean inlet velocity. An auxiliary simulation is performed with S3D in which a homogeneous isotropic turbulence field is generated using the method described by Rogallo, 1981 based on a prescribed Passot–Pouquet energy spectrum (Passot and Pouquet, 1987) that satisfies continuity. The turbulence field evolves from the imposed spectrum and the developed flow is characterized by turbulence intensity, \( u' / U^p_j = 0.35 \), and an integral length scale, \( l_{11}/D = 0.30 \), such that \( u' \) and \( l_{11} \) match the measured values of \( v' \), and \( l' \) from the experiment. The resulting field is then filtered such that it smoothly transitions to zero outside of the jet by multiplying the velocity
fields by the same hyperbolic tangent function used for the mean velocity. Employing Taylor’s hypothesis, velocity fluctuations are superimposed on to the mean inlet velocity. The initial conditions for the simulations are specified by the solution of a one-dimensional flame calculation from OPPDIF (Lutz et al., 1997). Subsequently, a laminar counterflow flame is simulated until the initially imposed conditions are washed out, before turbulence is injected.

4. Results and Discussion

The turbulent premixed flame topology depicted in the cartoon of Fig.1 is shown in more detail from the OH-LIF measurements in Fig. 2a. The images in Fig. 2 are rotated 90 degrees counterclockwise with respect to the schematic in Fig. 1 such that the streams of premixed reactants and hot combustion products are emerging from the left-hand side and right-hand side of the images, respectively. The topology of the lean \( \text{H}_2/\text{air} \) premixed flame is similar to some of the turbulent \( \text{CH}_4/\text{air} \) premixed flames studied in previous work (Coriton et al., 2013). In the images of Fig. 2a, a high \( \text{OH-LIF} \) signal is measured in the turbulent premixed flame reaction zone, whereas a significantly lower and nearly uniform \( \text{OH-LIF signal} \) is measured in the counterflowing combustion products. The regions with the largest \( \text{OH-LIF} \) signals indicate the location of the turbulent premixed flame, which is stabilized between the counterflowing reactant and product streams. The flame fronts appear severely corrugated from interaction with the turbulent flow field.

Figure 2b is a complementary set of images of the instantaneous OH mass fraction on the spanwise mid-plane from the DNS, chosen to highlight similar topological features as found in the experiment. Qualitatively the DNS images show the same level of flame wrinkling, corrugation and curvature as the experimental images. Regions of low OH concentration delineate extinguished regions and pockets of significant local extinction are evident in both the DNS and experiment. Furthermore, the time-resolved DNS data indicates that these extinction regions reignite resulting in the localized flame recovery over a much smaller time span compared to the interval between two successive experimental snapshots. Such events, being spatially and temporally intermittent, are better resolved in the DNS even though the total temporal duration of the DNS data is computationally limited. The experiments, which were designed to provide ensemble statistics from temporally uncorrelated single-shot measurements, do not track the temporal evolution of these events.

a)
Using the time-resolved three-dimensional results from the DNS, we analyze the dynamics of an extinction event. Figure 3 shows simultaneous snapshots of the heat release rate, normalized by the peak heat release rate for a freely-propagating premixed flame, (Fig. 3a), the magnitude of vorticity (Fig. 3b) and the scalar dissipation rate (Fig. 3c), displayed in the spanwise mid plane. The scalar dissipation rate is defined as $\chi = 2D_T|\nabla Z|^2$ where $Z$ is the mixture fraction, defined as a linear combination of the elemental mass fractions based on Bilger’s definition, (Bilger, 1988), and $D_T$ is the local thermal diffusivity. In Fig. 3a, the heat release rate in the upper right corner of the flame is much higher than at the bottom part (Fig.3a) and the portion of the flame front in the bottom of the images is undergoing local extinction, as indicated by the low heat release rate rates. Local extinction takes place along the surface of the mixing layer between the counterflowing jets, in agreement with previous experimental observations in methane/air flames, (Coriton et al., 2013). The location of the mixing layer can be identified as the boundary that separates the turbulent flow field, characterized by high levels of vorticity magnitude, from the opposed laminar stream of combustion products, which have very low vorticity. Close inspection of the vorticity magnitude and scalar dissipation rate fields reveals the extinction mechanism as follows. As the turbulent motions continually impinge upon the flame it is convected downstream towards the counterflowing products side of the mixing layer, and it extinguishes due to the lower-temperature and higher scalar dissipation rate conditions it encounters there. During extinction the flame zone is diluted by the product stream, leading to depletion of radicals in the reaction zone. This pattern repeats itself periodically. As the sequence evolves, the hole does not recover, but instead, is convected out of the counterflow domain.
Localized quenching never leads to complete blow-off of the flame in either the experiments or DNS. Instead, the extinguished regions are either convected out of the counterflow domain or, if their residence time is sufficiently long, the quenched regions reignite. Two separate mechanisms of flame reignition are identified: 1) by propagation of an edge flame over the extinguished area, or 2) by auto-ignition of premixed reactants in contact with hot products from the bottom stream, whereby, an ignition kernel forms and rapidly expands over the extinguished region.

The case of reignition by flame propagation is illustrated in the temporal sequence in Fig. 4 where the heat release is plotted, normalized by the peak heat release rate, for a freely-propagating premixed flame. At the beginning of the sequence (Fig. 4a), the lower portion of the flame is entirely extinguished along the mixing layer as indicated by very low values of heat release rate between the T = 300K and 1300K. On the upper part of the image in Fig. 4b, a premixed flame front starts extending toward the locally extinguished area and then reconnects with the gas mixing layer in Fig. 4c. The flame front propagates on top of rather than along the gas mixing layer. In Fig. 4d, a pocket of reactants has formed between the stream of counterflowing products and the locally generated flame products. The pocket of reactants is ultimately consumed by the flame front that ends up merging with the counterflowing products.

The second flame recovery mechanism of autoignition of an extinguished region is illustrated in Fig. 5 by a temporal sequence of the heat release rate shown in shades of brown on which the scalar dissipation rate is superimposed in shades of blue. The opacity of both heat release rate and scalar dissipation rate is also linearly varied in Fig. 5 such that their minimum values are fully transparent.

![Figure 3: Contours of instantaneous a) normalized heat release rate, b) vorticity magnitude (logarithmic scale), and c) scalar dissipation rate in the spanwise midplane. The domain extent is 6.6 × 8 mm².](image)

![Figure 4: Temporal sequence of the normalized heat release rate plotted in the spanwise mid-plane of the burner showing the reignition of a localized extinction by edge flame propagation. The white and red lines correspond to T = 300K and T = 1000K iso-contours, respectively. The domain extent is 12 × 8 mm².](image)
and maximum values fully opaque. At the beginning of the sequence (Fig. 5a) at time \( t_0 \), a large portion of the premixed flame is quenched near the upper right corner, highlighted by the white rectangle. Similar to the extinction event described in Fig. 3, occurrence of localized extinction coincides with large values of scalar dissipation rate along the mixing layer surface. A short time later at \( t = t_0 + 0.075\, \text{ms} \) (Fig. 4b), heat release starts to increase within the region of minimum scalar dissipation rate (white rectangle). Subsequently, at \( t = t_0 + 0.174\, \text{ms} \) (Fig. 5c), the heat release rate increases further and a premixed flame front has re-established itself in the previously extinguished region in Fig. 5a. The three-dimensional view indicates that re-ignition does not occur because of edge flame propagation; instead, ignition occurs by mixing of reactants and hot products. The flame may also benefit from back-support of heat from the counterflowing hot product stream, (Richardson et al., 2010).

![Figure 5: Volume rendering of the instantaneous heat release rate and scalar dissipation rate during an autoignition event. The domain extent is 6.6 × 8 × 8 mm.](image)

To examine the localized auto-ignition in further detail, we show in Fig. 6 a cross-section through the volume of heat release rate and scalar dissipation rate from Fig. 5c. The cross-section is selected in the spanwise plane and it is offset by 1.6 mm from the burner centerline. Local extinction indicated by the reduced heat release rate in the lower right corner of Fig. 6a is correlated with locally high scalar dissipation rate. In the middle of the images where the iso-contour of scalar dissipation rate forms a cusp towards the reactants, an ignition kernel has formed and is developing into a premixed flame front. At the tip of the cusp the scalar dissipation rate has decreased and heat release rate rises. Further analysis of the coupling between detailed chemistry and transport is necessary to understand the structure and time scales of the localized auto-ignition events.

![Figure 6: Contours of instantaneous heat release rate and scalar dissipation rate at \( t = t_0 + 0.174\, \text{ms} \) in a spanwise plane 1.6mm off the midplane. Domain extends: 6.6 × 8 mm².](image)

5. Conclusions
The dynamics of localized extinction and re-ignition in a highly turbulent lean premixed hydrogen-air flame were investigated in a joint numerical and experimental study. The turbulent flame was stabilized in a counterflow with a stream of fresh reactants opposing a second stream of stoichiometric $H_2/air$ combustion products in thermochemical equilibrium at 1475K. OH-LIF measurements indicated that, although combustion was stable, the turbulent premixed flame fronts experience a large frequency of localized extinction. DNS of the same burning conditions revealed further details on the mechanisms of extinction and re-ignition. Localized extinction correlated with increased values of the scalar dissipation rate along the gas mixing layer formed by the counterflowing jets. Re-ignition followed localized extinction occurred by two mechanisms: re-ignition by edge flame propagation or auto-ignition of fresh reactants mixing with the counterflowing products. Further work is needed to comprehend the extinction and reignition processes in details.

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