Influence of fuel type on advective heat flux and extinction scalar dissipation rate in negative edge flames

Kathryn R. Gosselin\textsuperscript{1}, Kristin M. Kopp-Vaughan\textsuperscript{2}, Michael W. Renfro\textsuperscript{1}

\textsuperscript{1}Department of Mechanical Engineering, University of Connecticut, 191 Auditorium Road, U-3139, Storrs, CT 06269-3139
\textsuperscript{2}Pratt and Whitney, 400 Main Street, East Hartford, CT 06118

In turbulent combustion, such as that encountered in a gas-turbine engine, regions of locally high strain may cause a flame hole to develop in the reaction sheet. The edges of the hole caused by this local extinction point can be characterized as forwardly propagating if they move in the direction of unburned fuel and air or negatively propagating if they move in the direction of products. The hole itself may close if the forward propagation is relatively fast, or it may grow and lead to global extinction if the negative propagation is dominant. Although the forwardly propagating flame edge has been studied extensively in the form of lifted flames, the negatively propagating flame edge has received less attention experimentally, due to its transient nature. In this work, a counterflow flame geometry was used to produce negative edge flames. This burner, which has been previously characterized, utilizes a high-velocity coflow to induce stable off-axis extinction due to an increase in scalar dissipation rate. Previously, it was found for methane flames that advection through the flame edge increased the extinction scalar dissipation rate as compared to extinction on the centerline. The flame edge scalar dissipation rate was correlated to the centerline extinction value, but since advection is a function of both the local velocity and temperature gradients, the correlation depends on details of the flame including its local velocity at the reaction sheet. Additionally, at low velocities, thermal and species diffusion through the flame edge played a larger role. The current paper describes an experimental and numerical study to extend the previous analysis to additional fuels in an effort to examine the impact of varying diffusivities on the local extinction scalar dissipation rate. The flame stability as a function of velocity and composition has been investigated for ethane and hydrogen, supplementing previous results for methane. The conditions leading to stabilization of a negative edge flame indicate that the flame edge is more robust for ethane and hydrogen as compared to methane, suggesting that the role of advection at the edge is even stronger than previously reported for methane edge flames. Results from the numerical simulations are examined to calculate this advective heat flux component.

1. Introduction

The stability of turbulent, non-premixed flames is of interest due to their use in a variety of applications. Such flames are susceptible to wide variations in induced strain and scalar dissipation rate due to velocity fluctuations. In regions of large concentration gradients, this can result in local extinction forming a hole in the flame sheet. This local extinction can either progress to global extinction if the hole size increases, or the hole can close creating an unbroken flame sheet. The role of induced strain in both local (Watson and Lyons, 2000; Favier and Vervisch, 2001; Rolon et al., 1995) and global extinction (Shih, 2009) has been shown by several investigators.

In order to understand the behavior of a local extinction point, a flame hole may be represented as a stationary hole in a nonpremixed flame sheet with bulk in-plane flow, as seen in Fig. 1. Along its perimeter, the flame sheet edges interact with partially-premixed air and fuel in the hole, forming three distinct regimes. The first of these is the forwardly propagating flame edge, denoted by (A), in which the local gas velocity brings unburned, premixed air and fuel into the flame edge. Forwardly propagating edges, which may be seen in lifted flames, represent a local flame propagation process, due to a low local scalar dissipation rate. Conversely, a negative edge flame, denoted by (B), receives burned products from the flame sheet due to the direction of the local velocity. It is subject to a high scalar dissipation rate, and is therefore a local extinction process. The stationary flame edge, denoted by (C), exists where there is no net advective
flux through the flame edge. The three edge types were predicted by Buckmaster (1996), although this work did not allow for variations in strain rate or scalar dissipation, preventing detailed analysis of their influence.

A forwardly propagating flame edge manifests in a lifted flame, which can be easily studied in the laboratory (e.g., Kioni et al., 1999; Kioni et al., 1993; Puri et al., 2001; Qin et al., 2002; Lee et al., 2003). In particular, Pleasing et al. (1998) used a simple axisymmetric burner with coflow to stabilize a lifted laminar methane flame and studied various flow conditions using laser techniques. These measurements, in conjunction with numerical simulation, found heat exchange among the branches of the triple flame as well as heat loss near the triple point were significant influences on flame stability.

The negative edge flame, however, does not lend itself well to evaluation in a turbulent environment. Laser techniques have been used to observe local extinction behavior in turbulent jets (Boxx et al., 2009) and estimate strain rates in these regions (Hult, 2005). Similarly, both Pantano (2004) and Sripakagorn et al. (2004) used direct numerical simulation to examine the effect of scalar dissipation rate on local extinction events in turbulent jets. While these numerical simulations allow a more detailed study of flow conditions at the flame edge, the extinction events are limited to those stochastically produced by the flow fluctuations, thus the location and timing of extinction must be captured during a transient simulation.

Several attempts have been made to induce and capture negative edge flame behavior experimentally, including by Santoro et al. (2000) and Amantini et al. (2007), who induced extinction on the centerline of a counterflow burner and captured both positive and negative flame edges as the flame rapidly receded to the outer edge of the burner. Similarly, work by Cha et al. (2006) utilized a counterflow slot burner in an attempt to replicate the simulations of Daou et al. (2002). Both the experimental and numerical works were able to produce positive and negative flame edges. The latter was observed in cases of high volumetric heat loss at both high and low strain rates, suggesting heat loss as a contributing factor to this phenomenon. However, the transient nature of these experimental methods precluded detailed measurement of local conditions at the negative flame edge.

In an attempt to create a stable negative edge flame, Shay and Ronney (1998) intentionally misaligned a counterflow slow burner. The resultant stationary edge was found in a region of strain lower than that required to produce global extinction in a spatially uniform flow field. However, the geometry of the burner produced a gas flow that was predominantly parallel to the flame, making it experimentally equivalent to a stationary edge, as in Fig. 1(C). Carnell and Renfro (2005) demonstrated that a stable negative edge flame may be successfully created in a counterflow burner and outlined the conditions required for stabilization. Similarly, Yang et al. (2009) constructed a double-slit counterflow burner in which various fuel and oxidizer arrangements were used to create a variety of stable local extinction points. They further quantified the stable flow regimes and correlated propagation speed to the local Karlovitz number.

A subsequent numerical study by Carnell and Renfro (2006) examined the energy balance at the flame edge for a methane diffusion flame in order to assess the relationship between the advective energy flux and the scalar dissipation rate required for extinction. This paper extends that work to other fuels and further analyzes the influence of advection through the flame edge.

2. Methods

The experimental setup consisted of a counterflow burner with a central nozzle including a 20-mm inner diameter and a 2-mm wall surrounded by a coflow with a 48-mm inner diameter. A cross section is shown in Fig. 2. Aluminum honeycomb was used to straighten the flow within each nozzle. A water jacket, which protruded above the burner edge and formed a small lip (2.5 mm high by 14 mm wide), was used to cool the burner surface. The nozzles were fixed in
place 15 mm apart for all measurements reported here. Choked orifices of various sizes were used to control flow through each of the nozzles.

The top inner jet consisted of a low velocity mixture of fuel – hydrogen, methane, or ethane – diluted with nitrogen, while the bottom inner jet consisted of only air. This configuration, in the absence of coflow, produced a traditional counterflow diffusion flame. Rather than a nitrogen guard flow, the outer nozzles issued another fuel/nitrogen mixture from the upper nozzle and air from the lower nozzle, but at a higher velocity than the inner nozzles. Similar to previous studies that used a high-velocity jet to initiate centerline extinction (Santoro et al., 2000; Amantini et al., 2007), this coflow increases the radial strain rate, which in turn causes extinction. A range of velocity ratios, denoted by the ratio of outer velocity to inner velocity, were measured. A complete detailed description of the experimental setup may be found in the previous work of Carnell and Renfro (2005).

The axisymmetric computational domain, shown in Fig. 2, is similar to the geometry of the experimental burner. A burner separation of 15 mm was chosen, and the burner nozzles were modeled as velocity inlets with uniform velocity and species profiles. The velocity inlets and the walls representing the lip of the cooling jacket and the small section of wall between the inner and outer nozzles were fixed at 300 K. The cooling jacket forms a lip of 2.5 mm above the nozzle, and it extends 14 mm beyond the outer nozzle. The outflow was modeled as a constant pressure outlet.

The resolution of the mesh was divided into three regions: first, a coarse mesh with a resolution of 250 µm for the cool, non-reacting flow near the nozzles, then a second mesh with a resolution of 125 µm, centered around the physical midpoint of the burner, and finally a fine resolution mesh with a resolution of 62.5 µm, centered around the heat release zone, which varied based on the fuel used.

A steady, segregated, axisymmetric, implicit solver (Fluent v. 14.0) was utilized for the numerical simulations. One-step reaction models were used; the rate exponents and pre-exponential factors used for each fuel are shown in Table 1, along with the activation energies used to calculate the volumetric reaction rate, \( \dot{\omega}'' \). One-step models are not expected to quantitatively predict extinction behavior, since they are known to under-predict parameters such as flame speed in certain conditions (Westbrook and Dryer, 1981); however, one-step chemistry should sufficiently capture the trends of interest.
to this work as shown for methane flames by Carnell and Renfro (2006). Simulated temperature contours for all three fuel types with a negatively propagating edge flame are shown in Fig. 3. Full details of this numerical formulation may be found in (Carnell and Renfro, 2006).

Table 1: Pertinent one-step mechanism data used in two-dimensional simulations

<table>
<thead>
<tr>
<th>Fuel Type</th>
<th>Rate Exponent – Fuel</th>
<th>Rate Exponent – Oxidizer</th>
<th>Pre-Exponential Factor</th>
<th>Activation Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>0.2</td>
<td>1.3</td>
<td>2.119×10^8</td>
<td>2.027×10^8</td>
</tr>
<tr>
<td>Ethane (Westbrook and Dryer, 1981)</td>
<td>0.1</td>
<td>1.65</td>
<td>6.186×10^9</td>
<td>1.256×10^8</td>
</tr>
<tr>
<td>Hydrogen (Fluent, 2009)</td>
<td>1</td>
<td>0.5</td>
<td>1.8×10^13</td>
<td>1.464×10^8</td>
</tr>
</tbody>
</table>

For the two-dimensional cases analyzed, uniform fuel mixtures were used in the inner and outer nozzles, the values of which are shown in Table 2. A velocity ratio of 3:1 (\(S_c:S_l\)) was chosen based on the agreement in extinction behavior between simulations and experiments for these cases, as seen in Fig. 4. An inner nozzle velocity of 18 cm/s was chosen for all three cases.

In order to examine heat transfer through the extinction point, simulated velocities, temperatures, species concentrations, and various other properties were exported for post-processing. At each node, the mixture fraction, \(Z\), was calculated from the method developed by Bilger and Stárner (1990)

\[
Z_{BLGR} = \frac{2Y_c/W_c + \frac{1}{2}Y_H/W_H + (Y_o^c - Y_o)/W_o}{2Y_c/W_c + \frac{1}{2}Y_H/W_H + Y_o^c/W_o}
\]  

where \(Y_i\) are the elemental mass fractions of carbon, hydrogen, and oxygen, \(W_i\) are the elemental atomic masses, and \(Y_i^c\) and \(Y_i^f\) are the elemental mass fractions in the oxidizer and fuel streams, respectively.

Centerline extinction behavior was determined using OPPDIF (Lutz et al., 1997), which utilized the following detailed mechanisms: GRI Mech 3.0 (Smith et al., 1999) for methane, the San Diego Mechanism (Saxena and Williams, 2007) for ethane, and Li et al. (2004) for hydrogen.

3. Results and Discussion

Extinction stability results, both experimental and simulated, for the three fuels of interest are shown in Fig. 4. Centerline extinction refers to the minimum fuel content required to sustain a standard counterflow flame, which is produced by using only the inner nozzles of the burner. These numerical results were obtained using OPPDIF with detailed chemistry. The additional data points, labeled by the outer to inner nozzle velocity, indicate the fuel fractions at which the flame transitions from a negative edge flame to a standard counterflow flame at a given inner nozzle velocity. These numerical results were obtained using Fluent with one-step chemistry. Previous studies (Carnell and Renfro, 2006) found that the outer nozzle fueling had minimal impact on extinction limits, thus the outer nozzles were held constant at 20%, 10.7%, and 9.4% fuel by volume, for methane, ethane and hydrogen cases, respectively. The inner fueling was gradually increased until the flame exited the burner, and this value was recorded.

Figure 4 shows extinction limits for all three fuels. Although there are quantitative differences between the experimental and numerical extinction limits due to the use of 1-step chemistry, the simulations are able to capture the trends for stabilization of negative edge flames. In the case of methane, the extinction flame region is bounded on the low end by
Figure 4: Negative edge flame stability limits for (a) methane, (b) ethane, and (c) hydrogen. Plots on the left are experimental results, while those on the right are numerical results.
centerline extinction, as expected. However, the negative edge limits for ethane and hydrogen are both below the centerline extinction limit, indicating that the edge flame is more robust that the flame on the centerline. This is consistent with the observation by Carnell and Renfro (2006) that showed advection through the flame edge supports the flame and extends its extinction limits. However, for ethane and hydrogen, this effect is exaggerated as compared to the previous methane results.

Individual terms of the steady energy equation

\[
0 = -\rho c_p \left( V_\text{a} \frac{dT}{dr} + V_\text{a} \frac{dT}{da} \right) + \lambda \left( \frac{d^2 T}{dr^2} + \frac{d^2 T}{da^2} + \frac{1}{r} \frac{dT}{dr} \right) + \frac{d\lambda}{dr} \frac{dT}{dr} + \frac{d\lambda}{da} \frac{dT}{da} - \sum_i \nabla h_i \cdot \mathbf{J}_i + \omega'' \Delta h
\]  

(2)

were calculated along the mixture fraction contour determined by the value at the point of maximum heat release. All local properties and derivatives were calculated via a third-order fit to the closest 6 cells. The residual of these energy budgets is less than 1% of the heat release in each case.

Figure 5 shows the radial energy budget arising from the terms of Equation 2. In each case, the radial geometry term, \( \lambda \frac{d\lambda}{dr} \), is negligible, indicating that the radial nature of the burner has little effect on the extinction behavior. That is, an extinction front stabilized in a non-radial environment would behave similarly. The effects of variable conductivity, \( \frac{d\lambda}{dr} \frac{dT}{dr} \) and \( \frac{d\lambda}{da} \frac{dT}{da} \), are also negligible, as well as the effect of species diffusion, \( \sum_i \nabla h_i \cdot \mathbf{J}_i \), since the rate of diffusion is negligible in comparison to the gas velocity within the flame. Therefore, the energy balance can be simplified to the following expression:

\[
-(V \cdot \nabla T) + \left( \frac{\lambda}{\rho c_p} \nabla^2 T \right) + \left( \omega'' \Delta h \frac{\rho c_p}{\rho c_p} \right) = 0
\]  

(3)

In a negative flame edge, the velocity through the edge aligns with a negative temperature gradient, such that the advection term, \( V \cdot \nabla T \), negative. Thus, the advection and heat release act as energy gains to balance the thermal diffusivity, \( \frac{\lambda}{\rho c_p} \nabla^2 T \), which is negative. This suggests that a higher rate of thermal diffusion is required for extinction as compared to cases without advection, due to the sign of the advection term.

In each case, heat production from reactions and axial diffusion both peak prior to the extinction point, after which point radial advection becomes the dominant source of energy gain. In both methane and hydrogen, both axial advection and radial diffusion have slight impacts on the energy budget through the extinction zone; however, in ethane flames, radial diffusion appears to be negligible.

In order to analyze the impact of advection through the extinction point, the energy budget was analyzed at the point of maximum heat release. This may be considered a marker for extinction because it indicates that the scalar dissipation rate has reached a point where the reaction rate can no longer increase to keep up with thermal diffusion (Carnell and Renfro, 2006). The results, shown in Table 3, indicate the advection through the negative edge may strengthen the flame. Methane, which showed the smallest extension to the stability limits for the cases tested, has an advection to heat production ratio of merely 1.92%, while ethane, which showed the greatest increase in stability, has a ratio of 9.25%. This may be due to the temperature gradient term, which is almost twice that of methane. Increased strain at the edge of the inner nozzle causes extinction and a rapid temperature decrease, which induces advection into the flame edge. Ethane experiences a more extreme temperature gradient under identical strain conditions, causing increased advection through the flame edge, which strengthens the flame considerably in comparison to methane. Hydrogen experiences a similar phenomenon, although the extinction limits are extended slightly less than ethane.

Table 3: Energy budget terms at extinction point

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Peak Heat Production [W/m³]</th>
<th>Radial Advection [W/m³]</th>
<th>Advection to Heat Production Ratio</th>
<th>( V_r ) [m/s]</th>
<th>( \frac{dT}{dr} ) [K/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>4.74×10⁸</td>
<td>9.22×10⁶</td>
<td>1.92×10⁻²</td>
<td>1.73</td>
<td>-2.11×10⁴</td>
</tr>
<tr>
<td>Ethane</td>
<td>1.46×10⁸</td>
<td>1.35×10⁷</td>
<td>9.25×10⁻²</td>
<td>1.21</td>
<td>-3.82×10⁴</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>1.49×10⁸</td>
<td>8.35×10⁶</td>
<td>5.58×10⁻²</td>
<td>0.78</td>
<td>-2.68×10⁴</td>
</tr>
</tbody>
</table>
4. Conclusions

Extinction limits for an axisymmetric, stabilized negative flame edge were studied using both experimental and numerical methods. Previous work focused on methane flames, while ethane and hydrogen were included in the present study. Although local extinction edges in flames utilizing methane have been shown to be supported by advection through the flame edge, those utilizing ethane and hydrogen showed even stronger extension of the extinction limit due to advection. Ethane and hydrogen edge flames were able to burn stably at fuel fractions well below the centerline extinction limit. Additionally, a radial energy budget through the extinction point was determined from numerical results. All fuels showed similar trends in the role of advection while quantitative differences between the fuels could be characterized.

References


Figure 5: Simulated energy budgets through the negative flame edge for (a) methane, (b) ethane, and (c) hydrogen.