Abstract

WANG, WEI. Investigation of Turbulent Lifted Jet Flame Stabilization Using Experimental Methods and Simulations. (Under the Directions of Dr. Kevin Lyons and Dr. Tarek Echekki).

The stability and structure of lifted jet flames are studied experimentally and computationally. A high speed charge-coupled device (CCD) camera with an intensifier system is used for the methane air lifted jet flame base visualizations. CH* distributions in reaction zones at different Reynolds (Re) conditions have been recorded. Reattachment and blowout processes are investigated. It is found that the heat releases at the flame base always remain high and stable; whereas, it decreases significantly downstream. Also, the shapes of the flame base mimic a partially premixed condition. As the Reynolds number is increased, flame holes near the stabilization zone become more prevalent. These holes perturb the flame base and make it unstable. Throughout the reattaching transition, local high heat release at the flame base is responsible for the flame stabilization until the flame transitions to an attached flame. During blowout, heat release at the flame edge decreases gradually resulting in flame extinction.

The application of simultaneous particle image velocimetry (PIV) with flame chemiluminescence enabled the study of the velocity variations at the flame edges. The streamline divergences at flame edges not only indicate flame base positions, but also are consistent with the streamline patterns of triple or edge flames. The measurements find two velocities in flame edges are indicators of stabilizing flames. One is the flame edge velocity, which is close but larger than the corresponding laminar flame speed, and the other is the
flame propagation speed. The two velocities ratio averages are similar in magnitude to the theoretical estimate of the triple flame speed as the square of the density ratio across the flame.

In simulations, two DNS methods were used to study shear layer flames with some degree of chemical complexity and a transitional jet flame with simple chemistry. In the shear layer flame simulations, heat release rates exhibit triple flame structures. The sharp heat release gradients between flame edges and flames downstream are consistent with the experimental flame base visualization. The displacement speed profiles, as well as the streamline divergence characteristics, show that the flame base is always a triple flame shape during the unsteady flame evolution despite the flame structure distortion by the flowfield.

Another DNS simulation of a lifted jet flame under transitional flow also demonstrates the presence of triple flames at the leading edge of the lifted flames. Moreover, all the flame edges are located in the laminar flow region and their position fluctuations are hardly observed. Because of the characteristic of transition flow, flames at exterior edges are almost laminar and premixed lean flames persist further downstream. Meanwhile, towards the center of the jet, the rich premixed branch appears intermittently because of unsteady flow conditions and the presence of high shear.

Furthermore, the RANS method with the eddy dissipation model (EDM) is implemented to investigate the lifted jet flame structures. The mean values of the normalized flame index clearly show a triple flame structure with the lean premixed, the rich premixed, and diffusion branches. Both co-flow and free jet conditions show the velocity variations
through flame edge decreasing firstly then increasing significantly, which also support the triple or edge flame stabilization mechanism. That is also consistent with the experimental findings and the DNS simulations. The simulation lift-off heights agree well with the experimental results and the EDM model is very efficient to model lifted jet flames.
Biography

The author, Wei Wang, was born in Taiyuan, China. He received his Bachelor of Science and Masters of Science in thermal engineering from Huazhong University of Science and Technology, in Wuhan, China. In 2005, he came to North Carolina State University to pursue his doctorate.
Acknowledgements

I would like to thank my advisors Dr. Kevin Lyons and Dr. Tarek Echekki for their directions, help, patience, and encouragement during my study. Their guidance has been invaluable to me through this entire process. Also, I want to thank Dr. William Roberts and Dr. Tiegang Fang for their helpful comments and suggestions. Thank you to Dr. Daniel Grühn for serving on my committee.

Thank you to Hemanth Kolera-Gokula, James Kribs, Jeff Milles, Nancy Moore, Bhargav Ranganath and Fei Zheng for their help and suggestions on this research work.
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Chapter 1. Introduction

1.1 Motivation

Lifted jet flames are widely applied from both small and large scale industrial burners to various chemical processes. Therefore, they are of the fundamental interest in combustion science. In jet flames, the fuel and oxidizer are initially introduced as separate streams into a burner. The oxidizer is usually stationary or slowly flowing in the direction of the jet stream. Meanwhile, the jets are often injected with relatively high speed at a direction normal to the ambient flow. At higher fuel flow rates, the flame has a tendency to lift off from the burner rim.

The stability of lifted jet flames is a classic problem in combustion. Research on lifted flames is challenging because of the many physical processes that interact in complex ways. Such processes include the complex role of chemistry, turbulent and molecular transport in establishing the structure and dynamics of these flames, especially at the stabilization zone. With the development of laser diagnostic techniques and advanced numerical methods, the focus of turbulent jet flame research has been to understand the interaction between the flow and the chemical reactions. The structure of the flame may be influenced by turbulence, buoyancy, chemistry, heat release, mass diffusion, and heat transfer and the interaction between the various factors may not be fully understood. The complex interaction of these physical processes makes it so difficult to develop the fundamental principles of how turbulent flames behave and stabilize under lifted flame conditions. Furthermore, it is this lack of understanding that makes it difficult to properly model and thus predict important
quantities such as the levels of combustion efficiency and the level of pollutants produced by utility power generation systems and engines.

Given the importance of the lifted jet flame, the stabilization mechanism of lifted jet flames have been studied extensively both experimentally and numerically. A number of theories have been advanced to explain the mechanisms of stabilizations under lifted flame conditions; however, there is limited consensus on a single theory and more likely there is merit to every single one of them.

1.2 Literature Survey

1.2.1 Characterization of turbulent lifted jet flames

Characteristics of turbulent lifted jet flame are discussed from the perspectives of flow, reaction, and the interaction between them.

Eddies of different length scales are a feature of turbulence and the range of length scales are wide. Small-scale mixing of eddies may range from 0.1 to 10 mm. Mixing of fuel and oxidizer at the molecular lever is a prerequisite of combustion. Molecular interaction spatial scales are 1 to 10 nm. For turbulent jet flow, an unsteady shear layer forms near the nozzle inlet, which may transition into a complex 3D turbulent shear layer downstream at high jet Reynolds numbers. The complexity arises from the presence of a multitude of scales where energy is primarily transferred from the larger scales to smaller scales in a cascade that eventually results in kinetic energy dissipation at the smallest scales. Additional sources of complexity are the presence of different instabilities, which govern the scale of the large eddies.
According to Kolmogorov’s 1941 theory, during the process of eddy development the kinetic energy is transferred from large scales to smaller ones until the dissipation into internal energy is in a sufficiently small length scale. In the homogeneous isotropic turbulence, the kinetic energy spectrum $E(k)$ is proportional to $\varepsilon^{2/3}k^{-5/3}$ ($\varepsilon$ is energy dissipation rate and $k$ is wavenumber) within the inertial range.

In turbulent lifted jet flow, the mean momentum flow rate of round jet (with $r$ radius) is $\dot{M} = \int_0^\infty \pi \bar{r} \bar{U}^2 r dr$ where $\bar{r}$ denotes ensemble density averages and $\bar{U}$ is the Favre mean axial velocity. In turbulent lifted jet flow, $\dot{M}$ is conserved.

From the perspective of chemistry and the reaction, typical flame thicknesses are of the order of 10 to 100 $\mu$m. The nature of this involves multiple scales like turbulent flow. The coupling of multiple scales between combustion and flow are fundamental in the turbulent lifted jet flame.

In addition to the basic scalars for expressing the features of this combustion such as temperatures, reaction rates, and flame shapes, a very important quantity, the flame speed $S_F$, has not been well formulated due to the lack of understanding of physics of turbulent lifted jet flames. However, the flame speed can be measured in experiments and compared to laminar premixed flame speed $S_L$ or displacement speed $S_d$. Although lifted flames under consideration are primarily non-premixed, the leading edge structure of these flames is very complex and may feature a partially-premixed structure with characteristic propagation speeds.
It is also known that combustion has an influence on flow. Heat release was found to reduce the global entrainment rate, while buoyancy was found to increase it (Ricou and Spalding 1961; Becker and Yamazaki 1978). As a result, the centerline fuel concentration decays faster for a non-reacting jet than for a reacting jet (Takagi et al., 1981).

The interfaces between reactions and flow also express the characteristics of turbulent lifted jet flames. One is the Damköhler number (Da), defined as the ratio of reaction rate to convective mass transport rate or as the ratio of characteristic fluid time to chemical reaction time.

When $Da$ is low, products form in distributed zones within the large eddies, following the mixing of entrained reactants. When $Da$ is high, products form within thin zones around the outer edges of eddies and then get entrained into their cores. If $Da$, based on species $k$, is defined as (e.g., Echekki and Chen 2003),

$$Da = \frac{\dot{\omega}_k}{-\frac{\partial}{\partial x_j} (\rho Y_k V_{j,k})}$$

where $V_{j,k}$ and $\dot{\omega}_k$ denote a diffusive velocity in the $j$ direction and a net production rate of species $k$, respectively. In addition, Noble et al. (2006) scaled the residence time as $\frac{d}{U_{ref}}$, where $d$ and $U_{ref}$ denote a characteristic length and velocity scale, respectively. Then the Damköhler number was given by

$$Da = \frac{s_{\alpha}^2 d}{a U_{ref}}$$

Here, $\alpha$ is thermal diffusivity. Another basic but important variable is the mixture fraction $Z$, which represents the mass fraction originating from the fuel mixture side in the entire
mixture. Some quantities are developed to describe the lifted jet flame. A very common way of modeling turbulent non-premixed combustion is to apply the laminar flamelet concept by Peters (1986). In the modeling, the interaction between the flamelet and turbulence resides in the scalar dissipation rate, $\chi$, which is defined as

$$\chi = 2D|\nabla Z|^2$$

where $Z$ is the mixture fraction and $D$ is its mass diffusivity (usually equated to the local thermal diffusivity). The probability density function (PDF) of temperature and species mole fractions can be obtained with respect to $Z$ and $\overline{Z^2}$, where $\overline{Z^2}$ represents the mean square fluctuations of $Z$. All of these basic variables are fundamental in describing lifted jet flames.

1.2.2 Methods of investigating turbulent lifted jet flames

Both experimental and computational methods can be applied in investigating turbulent lifted jet flames. Using simulation methods, Reynolds averaged Navier Stokes equations (RANS) is simply a time or ensemble average of the governing equations where the variables are expressed in terms of mean and fluctuating components. The fluctuating components in the decomposition result in the so-called Reynolds stress terms in the momentum equations, and similar terms in the energy and species equations, all of which must be modeled.

Large Eddy Simulations (LES), based on the spatial filtering of the Navier-Stokes equation. In LES, the transient nature of large-scale “eddies” in reacting flows can be captured. Sub-grid scale turbulence must still be modeled, often by means of an effective diffusivity for momentum and scalar transport.
Direct Numerical Simulation (DNS) proceeds to the direct solutions without any model. The Navier-Stokes, energy and species continuity equations can be solved directly by discretizing the equations, applying a very fine mesh over the domain, and attempting to resolve all of the important length scales of the flow. DNS is the most rigorous method of computational fluid dynamics; but, it also comes with a large computational cost.

These general simulation methods such as RANS, LES, and DNS are dependent on combustion models, grid resolution, and so on. Simplified or detailed chemical reactions can be applied in the simulation methods. Among them, DNS is the most accurate method, all relevant time and length scales are resolved. But it is very costly and restricted to low Reynolds numbers (Re) and simple geometries. While both LES and RANS need a priori knowledge and examinations by experiments, LES is more accurate than RANS but still time consuming. In this dissertation, the RANS and DNS methods are both employed to investigate lifted jet flames.

Using the experimental approach, instantaneous measurements are possible using laser based diagnostics. The techniques, such as Particle Image Velocimetry (PIV), Planar Laser-Induced Fluorescence (PLIF) and Rayleigh scattering, as well as the images acquired from laser diagnostic experiments, reveal features invisible to the eye and enable deeper insight into the flame structure and dynamics. Reaction tracers, such as OH and CH, have enabled the possibility of assessing the strain rate and velocity on the flame surface quantitatively (Hasselbrink et al., 1998; Rehm and Clemens, 1998; Hasselbrink, 1999; Carter et al., 1998). Rayleigh scattering was used to measure the temperature (Dibble and
Hollenbach 1980), and laser Doppler velocimetry (LDV) and particle image velocimetry (PIV) were applied to measure the velocity and turbulent properties (Takagi et al., 1981). Various planar laser-induced fluorescence (PLIF) techniques have been applied to image the reaction zone of jet flames. Furthermore, experimental accuracy is very important to interpolate data correctly. High-quality experimental data are invaluable to modeling efforts for use in comparing model results to real observations.

1.2.3 Stabilization mechanisms of lifted jet flames

Flame stability is critical for the safe operation of any combustion device. The lifted jet flame base is observed to be a bright wrinkled ring on the periphery of the fuel jet and fluctuates about a mean downstream location. The stabilization may involve the process of ignition, flame propagation, and extinction in the absence of a continuous external ignition source or bluff body. This section provides a review of the theories developed to understand lifted flame stabilization.

Pitts (1988) discussed experimental and theoretical findings on lift-off and blow-out phenomena. Since then, there have been many important contributions to address this stabilization mechanism. These papers have been reviewed by Burgess and Lawn (1999), Peters (2000), Cessou et al. (2004), Lyons (2007) and Lawn (2009). In this section, the stabilization mechanisms are classified by the premixed model, the extinction model, the large eddy model, the edge flame model, and the turbulence intensity model.

(1) The premixed model
Vanquickenborne and van Tiggele (1966) proposed that the fuel and oxidizer are completely premixed before the flame front. The flame gets a maximum burning velocity at the base of a turbulent lifted flame. Thus, the flame stabilizes where the stoichiometric mixture is formed. This oldest model originally applied the “premixed” idea into the jet diffusion flame and relied solely on premixed flame propagation phenomena. Later theories such as turbulence intensity and edge flame stabilization theories in fact expanded the “premixed” concept into turbulence mixing and partially premixed to define and scale mixing of fuel and oxidizer.

(2) The flamelets extinction model

It was Peters and Williams (1983) who initially formulated the model that the extinction of laminar diffusion flamelets by flame stretching determines the position of the flame front. They argued that the liftoff phenomenon is essentially an extinction process and the stoichiometric contours lie in a region of high strain that prevented the flame from reattaching to the nozzle. In their model, the flame is regarded as wrinkled laminar diffusion flamelets and no premixing is assumed. The flame stabilizes where the relevant scalar dissipation rate $\chi$ is below a critical value. But they did not address the existence of fluctuations in liftoff height.

Peters (1984) later showed that this parameter is much smaller at nearly all observed lift-off heights than the critical value for quenching. (At the small eddy scale, it may be argued that the viscous dissipation rate is the more fundamental parameter, since it is the motions characterized by the velocity gradients which give rise to the mixture fraction.
gradients, even though at the macro scale, they may be largely independent parameters.) Peters (2000) finally deduced that the extinction model is not valid and this appears to have been confirmed by the imaging measurements of Schefer et al. (1994), Starner et al. (1996), and Watson et al. (2003).

(3) The turbulence intensity model

Kalghatgi (1984) used the premixed model to derive an equation for a turbulent burning velocity $S_T$ that is proportional to the r.m.s of the axial velocity fluctuations $u'$.

$$\frac{S_T}{S_b} = b \left(\frac{u' l}{v}\right)^{1/2}$$

(1-4)

where $b$ is a constant and $\left(\frac{u' l}{v}\right)^{1/2}$ is the local turbulent Reynolds number. This model assumed that the turbulence intensity at the flame base controls the speed of the base.

(4) The large eddy model

Broadwell et al. (1984) first saw re-entraining hot combustion products and air back into fuel rich jet. Their theory involved chemical reactions taking place in thin strained laminar flame sheets at the fuel-air interface and in the premixed pockets of entrained irrotational fluid. Miake-Lye and Hammer (1988) argued that the linear relationship between liftoff height and exit velocity is a consequence of the large-scale strain imposed on the flame surface by large-scale turbulent jet structures. They hypothesized that the flame propagates from one structure to its upstream neighbor along the stoichiometric surface until the strain between these two structures exceeds a critical value.
Su et al. (2006) described the flame base motion, in terms of the axisymmetric mode of large-scale organization of the mixing field. In Figure 1.1, time advances from left to right. The instantaneous stabilization point for each time is represented by a gray circle. In (a), the stabilization point is initially far from the centerline, and the flame advances upstream against the low axial flow velocity. This simultaneously requires that the flame move radially inward, to maintain a flammable mixture. Eventually, the local axial flow velocity becomes sufficiently high that the flame begins to recede downstream (b). When the trailing coherent structure, which brings higher fuel mole fractions, overtakes the flame, the stabilization point moves radially outward (c). As the flame moves downstream and outward, the flow axial velocity decreases, until the flame once again propagates upstream (d) and the initial situation recurs (e). This description emphasizes the primary role of large-scale flow organization. Small-scale fluctuations and turbulence are higher-order effects.
Then the large eddy stability mechanism can be summarized as: the flame must propagate from one large eddy structure to its upstream neighbor and is able to migrate to its upstream neighboring structure repeatedly to stabilize the reaction zone. Large eddies create intermittency in the properties of the turbulence, which affects the lift off height.

This model also claims that large eddies, rather than small-scale turbulent diffusion, present one mechanism by which flammable gas is found in the region of the lifted flame. In addition, jets formed from axisymmetric contractions are designed to give a very high velocity gradient in the initial shear layer (the ‘top hat’ velocity profile) and to generate rapid mixing in filaments that are then carried outwards by the vortex rings to provide a flammable mixture at the observed radius of the flame. However, these filaments are more sporadic in the case of a fully developed pipe flow jet and their significance for this case has not been proven.

(5) The edge flame theory

The edge-flame concept is rooted in the mathematics of idealized 2-D flame structures, which Buckmaster (2002) extensively reviews. It argues that the leading edge is partially premixed and thereby can propagate upstream against the local flow. The edge-flame concept is also consistent with the triple flame structures. Tracing back the triple flame, the particular interesting findings are Ruetsch et al. (1994) predicted velocity, reaction rate, and temperature profiles of a laminar triple flame in a co-flow arrangement with unity Lewis number. The basic structure is described using a triple point anchored at the base of the flame
and departing downstream from it are the lean and rich premixed branches and the trailing diffusion flame.

Previous investigations found that the speed of the triple flame is controlled by two parameters: the curvature of the partially premixed front determined by the dissipation rate at the leading edge and the heat release from the combustion. Increasing the dissipation rates reduces the flame speed. The heat release causes the deflection of the flow upstream of the flame front and has the effect of making the triple flame propagate faster than the fully laminar premixed front. It was found that even when the heat release modifies the mixture fraction gradient and the flame speed, the flow velocity at the flame base still remains in the same order of magnitude as premixed laminar flames.

They found that the flame can be stabilized in an oncoming flow whose velocity is greater than the laminar flame speed. Their simulations account for heat release which causes an increase in the velocity component perpendicular to the flame front. This redirection of the flow toward the centerline is accommodated upstream by divergence of the streamlines as the flame is approached. Because the streamlines are diverging ahead of the triple flame point, the velocity decrease to the laminar flame speed at the triple point and then rises downstream of the triple point to a value proportional to $\frac{\rho_u}{\rho_b} S_L$, where the subscripts $u$ and $b$ denote the unburned and burned gas conditions, respectively. In addition, they found that the maximum upstream speed capable of sustaining the triple flame is proportional to $\left(\frac{\rho_u}{\rho_b}\right)^{1/2} S_L$, the reaction rate profiles are cup-shaped resembling the premixed wings and temperatures are bullet-shaped resembling the diffusion tail.
The edge flame stabilization mechanism gets some research support. Müller et al. (1994) used a partially premixed flame propagation model and successfully estimated the lift-off height of turbulent flames. Muñiz and Mungal (1997) applied PIV at the base of a lifted flame and measured the instantaneous velocities at the flame base. They found that the flame base resides at low speed regions typically with $u_{base} < 3S_L$, where $S_L$ is the maximum laminar flame speed of the fuel-air mixture. Similar observations were made by Schefer and Goix (1998), which support the stabilization mechanism by turbulent leading edge flame propagation.

Also, Upatnieks et al. (2004) offered their results with the edge flame model. In their examined methane/nitrogen (77%/23% by volume) at Re= 4300 lifted turbulent jet flames, shown in Figure 1.2. The “hot” zone outlined by the 600K isotherm is argued to exist in its own low axial velocity, low turbulence region that diverges streamlines at the leading edge. They maintained that two propagation velocities of the edge flame are important. One is the actual burning velocity of the flame relative to the disturbed flow which is on the order of the laminar burning velocity. The second is the effective propagation velocity of the whole edge flame.
Figure 1.2 The experimental data of velocities fields diverging at the leading edge of the reaction zone (from Upatnieks et al., 2004).

Mansour and Joedicke et al. (2006) examined flame structures using a combined 4-camera technique for multi-reaction zones imaging. The technique combined highly advanced laser-based diagnostics tools, namely Rayleigh scattering, laser-induced predissociation fluorescence (LIPF) of OH, LIF of PAH, and LIF of formaldehyde (CH$_2$O). In Figure 1.3 and 1.4, the image data shows simultaneously rich, lean and diffusion reaction zones and supports the triple flame concept. The 3 reaction zones can be spatially resolved, providing essential information about their interaction and overall flame stability.
(6) Other models

Some researchers think the above 5 categories are not necessarily independent. For example, Kelman et al. (1998) argued that the lifted jet flame is stabilized from a sequence of partially premixed upstream propagation (condition 1) which evolves into a diffusion flame structure (condition 2). Then it is extinguished locally through a flame-vortex interaction from the jet structures (condition 3) and subsequently drops downstream fuel and air mix upstream to complete the cycle then repeating with condition 1, etc. Eickhoff (2005) pointed out that premix model and the edge flame model are actually cast in terms of the turbulent Damköhler number.

Figure 1.3 Simultaneous images from Mansour and Joedicke et al. (2006): (a) Rayleigh; (b) LIF-CH₂O; (c) LIF-PAH and (d) LIF-OH.

Figure 1.4 Shown from Mansour and Joedicke et al. (2006), Combination of the red contours illustrated in Fig 1.3.
In addition, other researchers investigate the role of auto-ignition in stabilization of lifted jet flames. Yoo, Sankaran and Chen (2009) performed DNS simulations of a three-dimensional spatially developing turbulent lifted hydrogen jet flame in heated co-flow with a detailed mechanism to determine the stabilization mechanism and the flame structure. Their result argued that auto-ignition in a fuel-lean mixture at the flame base is the main source of stabilization of the lifted jet flame. Downstream of the flame base, both rich-premixed and non-premixed flames develop and coexist with auto-ignition. From Lagrangian tracking of the flame base, they claimed that the position of the flame base moving cyclically is affected by the coherent large scale flow structure and the flame stabilization is determined by the balance between the local axial velocity and auto-ignition which favors hot environments with low scalar dissipation rate. However, this work only applied to heated co-flow. It is unknown in the normal temperature co-flow conditions.

1.3 Aims and Scope

In this dissertation, both experimental and simulation methods are used to identify the stability mechanism of turbulent jet lifted flames. Experiments focus on flame base traces and flame zone detection. Velocity variations are examined by a PIV method. On the simulation side, DNS and RANS are used to rebuild the lifted jet flames and investigate the flame structures and flow characteristics. Stable and unstable flames are studied with DNS methods. Co-flow and free jet flame structures are studied using the RANS method. All possible stabilization mechanisms are discussed based on the results and finally the lifted jet flame stabilization mechanisms are summarized.
The aims of the research can be summarized as follows:

- To visualize flame bases using a high speed camera with an identifier and study the flame base shape using CH radical distributions.
- To detect the flame zones and probe velocity variations at flame bases using a simultaneous PIV experimental system.
- To study the implications for lifted jet flame stabilization from the experimental data.
- To investigate the flame structure evolutions through DNS simulations on an unsteady shear layer flame.
- To analyze the flame stability from a stable lifted jet flames with a transition phase with a DNS method.
- To study the flame structures under various configurations using the RANS approach.

Chapter 2 describes a high speed camera system with an intensifier and visualization of flame bases using CH\(^*\) images. In Chapter 3, a PIV system is setup to measure the velocities at flame bases from a free lifted jet flame and evaluate the stabilization mechanism.

The results of a direct numerical simulation on a shear layer flame at different times are given in Chapter 4. Chapter 5 describes the simulation on a stable 2D lifted jet flame with a relatively low, yet transitional, Reynolds number of 2500. The stabilization mechanism is studied. The focus of Chapter 6 is the RANS simulations of lifted free jet and co-flow jet flames. Also stabilization principles are discussed. Conclusions and recommendations for future work are presented in Chapter 7.
Chapter 2. Visualization of Turbulent Jet Flame Bases

2.1 Introduction

In non-premixed combustion, the flame structures are quite different from those of premixed flames because the mixing process plays a dominant role for flame stabilization and significantly contributes to the shape of the reaction zones (Meier et al., 2005). In practical combustors like gas turbines, the prototypes are typical lifted jet flames. But neither pure premixed nor pure non-premixed flames are usually found (Meier et al., 2005). In this kind of combustion, fuel and oxidizer are initially separated in lifted jet diffusion flames. The structure of the bases of lifted jet diffusion flames is expected to be complex.

The non-reacting lift off region with turbulent lifted flames gives fuel and oxidizer time and space to mix before encountering the flame zone. The zone corresponding to the lift-off height involves a degree of mixing between fuel and oxidizer, resulting in a partially premixed flame structure at the leading edge of the lifted flame. It is possible that the flame base includes both premixed (lean, rich) and diffusion flame structures. Also, premixed and diffusion flames can easily merge to broaden the reaction zone under jet flow impact. In addition to the presence of premixed and non-premixed flame branches at this leading edge, the effects of turbulence may play an important role in determining their structure and topology. Visualization of the flame base is necessary to investigate this hypothesis and it
may provide evidence of the extent of mixing and the structure of this base. It will also aid us to evaluate if the partially premixed or triple flame stability theory can explain the lifted jet flame stabilization.

Flame base shape visualization should delineate reaction zones reasonably well. Usually, CH$^+$ and OH$^*$ are considered as good candidates. But OH$^*$ can cause ambiguities in determining the flame surface owing to its slow removal by three body recombination reactions (Seitzman et al., 1990). It is only considered as an indicator of the region of burnt gases (Hanson et al., 1990) and is useful to separate the unburned mixture and the burned gas (Tanahashi et al., 2005). Contrary to OH$^*$, CH$^+$ is formed and removed by faster two body reactions and a good marker of the fuel decomposition region (Seitzman et al., 1990). It is produced at the flame front near the stoichiometric contour and has width narrow enough to represent the reaction zones (Mansour et al., 1998, Carter et al., 1998 and Donbar et al., 2000).

More recently, Choi et al. (2007) used DNS simulations and CH PLIF measurement methods to investigate the relationship between CH$^+$ and heat release rates. In their DNS simulations, even for the premixed flame in high intensity turbulence, the distribution of the local heat release rate coincides with that of the CH mole fraction. Their experimental results showed that CH PLIF intensity can represent the difference in the CH mole fraction due to the equivalence ratio. Their study implies that CH PLIF measurements can be applicable for the estimation of the local heat release fluctuations in turbulent flames. However, some researchers stated that the CH$^+$ cannot represent heat release very well (Lauer et al., 2010 and
Gordon et al., 2009). Gordon et al. (2009) suggested multiplying OH by CH$_2$O to represent heat release. Frank et al. (2005) used the product of CO and OH to calculate the forward reaction rate of CO + OH = CO$_2$ + H to mark reaction zones. Linteris et al. (2008) used flame areas to measure heat release. Despite this argument, it has been found that the integral heat release of the flame and the integral chemiluminescence emission of the species CH show an identical monotonic behavior (Lauer et al., 2010). Najm et al. (1998) showed the results from the laminar premixed flame computation using the PREMIX code, the peak of CH* concentration position is approximately 50 µm apart from the peak position of the heat release rate. This error is negligible, so CH* concentration position can be used to represent heat release in jet lifted flame experiments (Han, 2001). It is believed that the CH radical, which possibly represents most of the reaction zones, can provide deep insight in turbulent combustion (Han et al., 2000 and Choi et al., 2007).

In this experiment, the objectives are to investigate the flame base’s overall macroscopic shape and the shape differences between flame edges and flames downstream. Also, the CH* images are three dimensional data projected on the CCD 2D plane. The accuracy of the maximum heat release position is not important for this study. The CH* concentration profile can represent the entire flame energy distribution in the large length scale very well.

In this chapter, three different jet flames at Reynolds numbers based on the fuel jet inlet conditions (Re = 4800, 6400 and 8300) are captured by high-speed camera with an intensifier. Reattachment and blowout phenomena from a stable lifted jet flame are also
investigated. From the analysis of the flame base images, we conclude that lifted jet flame stability is a global phenomenon and flame base are partially premixed flames and their structure and topology play a unique role in the flame stabilization mechanism.

2.2 Experimental Setup

The experiments were performed at the Applied Energy Research Laboratory on the campus of North Carolina State University. The burner (schematic as Figure 2.1) provides fuel from a center nozzle and concurrent air flow. The fuel flow is controlled by a rotameter and then directed through a 3.5 millimeters (mm) diameter stainless steel pipe long enough to ensure fully-developed flow. The calibrated rotameter with ±5% accuracy is used to measure the volume flow rate of the methane entering the fuel pipe, from which the fuel velocity is calculated. The jet is seeded by 99.9% pure methane and there is no co-flow input.

The CH* emission is used to delineate the flame and is captured by a high speed camera with an intensifier. A Kodak EKTAPRO model 4540 high-speed camera is lens-coupled to an Imco ILS-3 intensifier with a 55 mm F1.8 UV-Nikkor lens. The system facilitates imaging at framing rates up to 4,500 frames per second and the maximum record time is 1 second. The CH filter is the central wavelength of 430 nanometer (nm) with a 10 nm full width half max. The Schott KV-418 color glass filter ensures that the CH chemiluminescence between 420 and 440 nm is transmitted while additional scattering is rejected. The image resolution is 256 by 256 pixels.
2.3 Result and Discussions

2.3.1 Typical flame base shapes

Because the two flame base conditions of partially premixed or only stoichiometric premixed were developed into the fully premixed stability theory and the edge flame theory, introduced in Chapter 1, it is very important to classify what the lifted jet flame base shape is. In this section, we investigate flame base shapes and compare them to the visual characteristics of laminar fully premixed and partial premixed flames. The fully premixed theory states that the lifted jet flame base is only stoichiometric premixed. Thus, the flame base must look uniformly thin. Otherwise, the flame front must contain other flame structures of partially premixed flames. However, the partially premixed theory claimed that the flame base is shaped like a leading edge including a triple (lean, rich and diffusion) flame structure or part of one. Therefore, the reaction zone in the flame base must look bold and thick, and it must have high luminance, while its adjacent downstream flame shows obvious gradients.

Figure 2.1 Schematic of the lifted jet flame image recording system.
A typical laminar premixed flame structure, diffusion and triple flame structure are shown in Figure 2.2. Although they are only luminous images, the edge of luminous regions are observed to coincide with the depletion of the original reactants (Borman et al., 1998).

![Typical laminar flames, diffusion flames and triple flames.](image)

(From Clarke et al., 2009) (From Hentschel et al., 2005) (From Kim et al., 2005)

**Figure 2.2** Typical laminar (a) Premixed flames, (b) Diffusion flames and (c) Triple flames.

Figure 2.2 (a) is a stoichiometric premixed methane air flame luminous region at ambient conditions of 298 K ±5K with fuel and air premixed in a pipe (reprinted from Clarke, A. et al., 2009). Flames attach to the burner at a low flow rate. Reaction zone are distributed in a uniformly thin manner. The total flame thickness is 0.89 mm and covers all reaction zones (Clarke, A. et al., paper). Figure 2.2(b) is a methane air diffusion flame luminosity image in a stationary and steady condition with fuel input from a pipe (Hentschel, J. et al., 2005). Upstream flames are thin but become thicker downstream, which means downstream flames have wider flame mixture fraction range. Figure 2.2(c) shows a typical laminar methane air triple flame luminous image (Kim et al., 2005). The flame shapes change with fuel mass fraction gradients, but the flame bases always maintain bold bright
appearance and have thick edges and the downstream trailing diffusion flames are dimmed. Furthermore, the overall flame luminous distribution trend remains consistent across the varying fuel mass fraction gradients. The energy distribution is clearly quite different; in other words, the gradients are obvious between the edge and downstream positions.

Figure 2.3 shows the typical CH\textsuperscript{+} distributions at three different Re numbers (4800, 6400, and 8300) in the experiments. The intensifier gain is set to 90%. The maximum image grayscales are around 241 which is less than the saturated value of 255. The images on the left are originals and the inlays show magnified flame edges with increased contrast. The images on the right are their corresponding grayscale distribution contours. From Figure 2.3, the CH\textsuperscript{+} densities get the highest values at the flame base and thus reflect the largest heat release. Downstream from the flame base, the CH\textsuperscript{+} density is globally reducing. The sharp gradient distributions of the CH\textsuperscript{+} look very similar to the triple flames in Figure 2.2(c), which also characterize highly non-uniform reaction zones with very large values at flame edges, smaller values downstream. Notice that when the Re number equals to 4800, the CH\textsuperscript{+} grayscales in some downstream positions are still high. This indicates that under the low flow rate condition, there are still stoichiometric flames downstream with both premixed and diffusion flame branches. It may also involve merging premixed and diffusion branches. As the Re number increases, the sporadic high values of the CH\textsuperscript{+} density no longer appear downstream, but the flame bases still retain the largest CH\textsuperscript{+} concentrations. This findings show that the flame base holds a very high amount heat release or energy, which can keep the flame stable and make the flame propagate downstream as well. This flame stabilization can
be explained by a global phenomenon and controlled by the flame base. Figure 2.3(a) shows the CH\(^*\) distributing non-symmetrically at the flame base. Two anchor-shaped edges stand at the left and right of the flame base. Figure 2.3(b) shows the high CH\(^*\) regions at the flame base merging, but there are islands with slightly smaller magnitudes than that of the main bulk. Figure 2.3(c) shows that the high CH\(^*\) density area on the flame base is shrinking and appears to be highly non symmetric; the separating flame islands at the flame base increase in number and decrease in size. These significant variations of the CH\(^*\) distribution at the flame base could be attributed to the turbulence effect which makes flow fluctuate more intensely as the Re number increases. This variation can reduce the flame base stability, but it is not strong enough to destroy the flame base stability and therefore the whole flame can survive.

In addition, in Figure 2.3 grayscale contours, the highest grayscales (occurring at the flame bases) are larger than the visualized maximum contour level (220). In fact, the maximum values, when probed, are around 241 in all the three cases. The magnitude of these maximum values indicates that stable lifted jet flames require a high and almost constant energy to stabilize the entire flame. Here, the visible flames are defined by a minimal grayscale value of 40. In all three cases, the flame base structures look like triple flames undergoing stretching or transformation. Therefore, the flame base can be called a partially premixed condition with a transformed triple flame structure. The entire flame gets the largest heat release at the flame base then propagates downstream.
Figure 2.3 CH\textsuperscript* distributions of lifted jet flame bases at (a) Re=4800, (b) Re= 6400, and (c) Re= 8300.
2.3.2 Flame holes

Under normal burning conditions, reactants diffuse toward the flame. They react and produce heat that is subsequently diffused away from the flame. This is required in order to maintain a temperature sufficiently high to ensure that the reaction remains continuously active. When the rate of strain is too large, the rate at which heat escapes exceeds the rate at which it is produced by chemical conversion and the flame is extinguished locally, forming flame holes. When the scalar dissipation is sufficiently large, the flame holes grow quite fast. No mechanism can oppose the expansion of the holes. On the other hand, when the scalar dissipation becomes small, the holes close. Flame holes are a normal phenomenon in lifted jet flames. There is sufficient evidence in the literature related to the presence of flames holes within the context of opposed-flow diffusion flames (Pellet et al., 1998; Lee et al., 2000) and lifted flames (Lyons et al., 2005). Lyons et al. (2005) reported experimental observations of local extinction characterized by flame holes that are close to the leading edge of lifted flame stabilization zone. These holes form their own edges, which can grow or shrink depending on the local dissipation rate field.

The relationship between flame holes and flame stability is discussed in this section. In contrast to previous work by Lyons and co-workers (see for example, Lyons et al., 2005), we adopt a different visualization strategy for the flame holes based on images of flame chemiluminescence, which maintain some of the 3D aspects of the flame structure. Flame holes are indicated in Figure 2.4 by dashed arrow lines. They are characterized by dark regions of limited to no chemiluminescence indicating the presence of local extinction. The
flame holes shown in Figure 2.4(a) at Re=4800 are regular round shapes and are located downstream from the flame base. Three consecutive snapshots of a flame hole at 2.22 ms intervals are shown to observe the evolution of this flame hole over time. The flame hole survives throughout the three periods and migrates downstream. This local extinction lasts some time, but it is not strong enough to degrade the flame stability (i.e. does not extend or growth to the stabilization zone). Also, this kind of flame hole is frequently observed downstream from the flame base. The left image of Figure 2.4(b) is a flame hole with Re=6400. It has an irregular shape and is located almost at the flame base. The hole obviously cannot survive for 2.22 ms as shown in the right image of Figure 2.4(b), which is taken after this time interval. The left image of Figure 2.4(c) shows two flame holes at the flame base which make one part of the flame base separate from the rest. The flame holes disappeared after 2.22 ms, which is shown in the right image of Figure 2.4(c). Note that the middle hole indicated by solid arrow lines is not a flame hole. It only appears because highly non symmetric flow at higher Re numbers makes the flame base shape extremely irregular. Thus, the typical ring shape of a round jet flame base in 3D is captured in the 2D image as the middle hole. We also observed that flame holes appear frequently at the flame base at Re=8300 and sometimes there are multiple flames holes as in the left images of Figure 2.4(c) and Figure 2.4(d). At other times, there is only one flame hole as in the middle and right images of Figure 2.4(d). A lone flame hole is not able to tear the flame apart while multiple closely packed flame holes potentially can. That indicates that high Re numbers lead to the flame holes becoming more aggressive to the flame base. In addition, Figure 2.4 shows that
flame holes would occur closer to the flame base and develop faster as Re number increases. Therefore, the flame holes would more severely impact the flame base structure, making it discontinuous, meaning that flame holes have a negative influence on flame stability.
Figure 2.4 Flame holes evolution at (a) $Re=4800$, (b) $Re=6400$, (c) $Re=8300$, and (d) Three examples of flame holes at flame base of $Re=8300$. 


The previous flame hole is gone

The previous flame holes are gone
2.3.3 Analysis of jet flame reattachment

When the jet inlet velocity is reduced to a critical value, the stable lifted jet flame cannot hold the lift off condition any longer and will keep propagating upstream until it attaches to the nozzle. Reattachment time depends on how much and how fast the jet inlet velocity decreases. In this reattachment process, a stable lifted jet methane air flame with a small lift off height underwent a quick jet inlet flow rate decrease. We did not probe the reattachment time but focused on how the flame base structures change.

Figure 2.5 shows the lifted jet flame reattaching procedures. During this period flames are much brighter than normal lifted ones, especially downstream. The intensifier gain cannot be set as high as 90% but instead is set at 80% to avoid damaging the intensifier. The maximum grayscale values in the entire flame are around 242 (less than saturated), which is very close to the value 241 seen in section of 2.3.1. Using this gain setting, the flame base grayscales are less than 242 but are still very readily recognizable. The inlays in Figures
2.5(b) through (f) are magnified flame base images to show the slope of the flame base. Figure 2.6 represents the corresponding flame base CH* grayscales of Figure 2.5. The largest grayscales at the flame bases were probed at 186, 186, 177, 173, and 169 in the 5 images of Figure 2.6(a) through (e), respectively. The dashed lines represent flame base slopes. The last image of Figure 2.6(f) has completely attached to the nozzle, meaning that there is no lifted flame base any more.

The time in Figure 2.5(a) is referenced as time zero. The dashed arrows are pointing at locally higher CH* density zones at the flame base. The contrast is increased in the inlaid image to better show the shape of the flame edge. In the corresponding grayscale contours of Figure 2.6(a), there are two regions at the flame base (left and right) that obviously have higher CH* densities. Figure 2.5(b) is taken 24.42 ms after Figure 2.5(a). Also, Figure 2.5(b) shows that the velocity gradients are steep and only a few pioneers at the flame base are moving and searching for new stable positions. Clearly, this behavior results in the left locally higher CH* value zone at the flame edge fading (in Figure 2.6(b)). Figure 2.5(c) shows some points at the left flame edge attaching to the nozzle after 36.63 ms and the velocity gradient distributions along the flame base are almost straight. Also, the left locally higher CH* value zone almost disappears (in Figure 2.6(c)) as the left flame base touches the jet tube. In Figure 2.5(d), after 51.28 ms, the flame base slope changes to a convex shape. Every point on the entire flame base has moved and the lagging points are catching up with the pioneers and thus the velocity gradients are rounded. The locally higher CH* density zone at the right flame base also starts to fade (in Figure 2.6(d)). Figure 2.5(e) continues the trend
of Figure 2.5(d) and the velocity gradient slope is almost flat. Finally, in Figure 2.5(f), the entire flame base reattaches to the nozzle and is stable. There is no obvious CH\textsuperscript{*} density distribution gradients until far downstream.

This reattaching process indicates the reattaching starts from very few points at the flame base then spreads to their neighbors. In addition, at the positions where the flame base finally attaches, the grayscales drop to only around 60 to 70. This is because CH\textsuperscript{*} is not only a function of reaction rate but also temperature. The reaction intensity goes down because of the reattachment and the temperatures decrease as well because of the heat transfer between flames and the steel pipe. Therefore, the CH\textsuperscript{*} density decreases significantly at the pipe rim.

According to the flame reattachment findings, the CH\textsuperscript{*} density always remains higher values at the lifted flame edges than their neighboring regions. The inlaid image of Figure 2.6(f) is CH\textsuperscript{*} distributions of the entire reattached flame. It shows that the CH\textsuperscript{*} density distributions downstream are even higher, which also appears at other times during the reattaching procedure. This may be due to the following reasons: first, under this low flow rate condition, large quantities of fresh fuel and oxidizer downstream can mix well and the mixture occupies a large space. Second, the high downstream temperatures make the combustion more complete than the upstream combustions and therefore even higher temperatures are reached downstream. Third, with the over ventilated flow, flames downstream interacted heavily. The CH particles do not easily disperse under the low flow rate. In contrast, they can deposit easily downstream.
The flame reattachment is summarized as follows: it is a transition process from a turbulent phase to a laminar phase. During the moving process, the flame base maintains higher heat release or more intense reactions than local downstream regions, but the CH* distribution gradients are not as sharp as the stable lifted jet flames in Section 2.3.1. The local higher CH* density domains will not be impacted until some part of the flame reaches the jet tube nozzle. After the flame reattaches, the lift off condition totally disappeared. Then the CH* or heat release distributes quite uniformly near the jet nozzle tip until more severe combustion zones appear far downstream. This corroborates an essential change from a lift off flame to an attachment flame. Therefore the lift off stabilization mechanism vanishes because of the change. Also, in the attachment flame, the CH* distributes as a laminar diffusion flame, low densities upstream and increasing gradually downstream, which is similar to Figure 2.2(b).
Figure 2.5 A typical reattachment from a stable lifted flame condition.
Figure 2.6 Flame bases grayscale contours of Figure 2.5.
2.3.4 Analysis of jet flame blowout

The conditions for blowout are directly related to the extinction mechanism. Broadwell et al. (1984) proposed that, the combustion ceases when the jet inlet velocity reaches a critical value. The extinction occurs because the flow is too fast to ignite the incoming fuel/air mixtures by entrained hot products. Miake-Lye and Hammer (1988) pointed to the primary role of large scale structures in facilitating hot product transport. Han and Mungal (2000) also offered observations on flame blowout and stated that the reaction zone is unable to counter-propagate against incoming reactants at blowout. Burgess and Lawn (1999), Brown et al. (1999), Dahm and Mayman (1990) and Montgomery et al. (1998) discussed related elements of flame blowout. A recent overview of this previous research in blowout is contained in Chao et al. (2004), Wu et al. (2006) and Aggarwal, S.K. (2009).

Differing from their analysis based on the extinction mechanism, in this experimental blowout analysis, we study the phenomena from the aspect of the flame base stability. Figure 2.7 shows jet flame blowout procedures and Figure 2.8 is the corresponding grayscale contours. In Figure 2.7, the images inlaid the up right corner show flame bases after contrast and brightness were increased. The inlays in Figure 2.7(a), (b), and(c) have a 40% contrast increase (from 50% to 90%), while the inlays brightness in Figure 2.7(d) and (e) was increased by 20% in addition to the contrast change. The blowout process started from a high lift off position (near to blowout condition), then it underwent a rapid jet inlet velocity increase. Similar to reattachment, we focused on flame base shape evolution during the flame blowout rather than probe the accurate procedure time. Even though the initial flame lift off
position is very high, the camera still cannot record the whole process because of the recording time and spatial range limitations (short) allowed by the camera/lens system. Thus, images were recorded some time after the blowout process started. The first image of Figure 2.7(a), referenced as time zero, is when the flame edge first appeared in the image recording window.

During the flame blowout process, the flame shape is like a flocculent cloud, which indicates flames accompany flame holes tightly. During 0 to 378.5 ms, the high contrast CH* concentration images of Figure 2.7(a) to (c) still show obvious gradients between flame bases and downstream flames. In the corresponding grayscale contours of Figure 2.8(a) to (c), if a visible flame value of 40 is selected (the same as in Figure 2.3), the heat release gradients between flame bases and downstream flames are \( \frac{200}{40} \), \( \frac{200}{40} \), and \( \frac{160}{40} \). After 422.5 ms, the gradients are sharply decreased. The brightness of the inlays in Figures 2.7(d) and (e) had to be increased; otherwise the figures would be all dark. In Figure 2.8(d), the corresponding gradient is around \( \frac{90}{40} \). In Figure 2.8(e), the maximum grayscale is 20, (the original image of Figure 2.7(e) is already dark), less than the required visual flame value of 40. Therefore Figure 2.7(e) and Figure 2.8(e) are only considered to be residual heat. Figure 2.7(f) images are totally dark and Figure 2.8(f)’s grayscale are less than 3, both indicate the residual heat is gone.

According to the analysis of Nancy et al., 2008, the flame blowout occurs at mixture fractions less than 5\% for methane air jet flames and all flames should be in lean conditions.
The heat dropped gradually in the flame base and therefore the heat of its propagating flame decreased as well. Even though the flame base energy continually decreases and stays in very lean conditions, flame characteristics such as the flame base shapes, flame zone heat release gradients and the phenomenon of flame islands are still very similar to the stable lifted flames in Section 2.3.1. However, the heat release gradients throughout the entire flame are decreasing.

The flame blowout can be explained as follows: with the increase of the incoming velocity, the flame base moves downstream where it could reside in a lower velocity gradient and thus a lower mixture fraction gradient region so that it could sustain increased incoming velocity. Obviously, the incoming velocity exceeded what the flame base can sustain and the entire flame blows out. During the blowout process, some lean mixtures of fuel and air can still be ignited at the flame base and the flame can propagate downstream for some time. But the combustion is too weak and lacks the supply of a reaction qualified mixture of fuel and oxidizer. This situation is getting worse as the entire flame moves downstream during the blowout process. Also, the reducing CH* grayscales shows that the flame energy is becoming weaker and temperatures are getting lower and, eventually, no gas can be ignited.

Based on the findings, the blowout is actually a process during which the flame base loses its stability gradually and cannot stabilize the whole flame any more. Finally, the entire flame is extinguished.
Figure 2.7 A typical flame blowout process.
Figure 2.8 Grayscale contours of Figure 2.7.
2.4 Conclusions

We conducted a series of methane air lifted jet flame experiments including stable conditions at three different Reynolds numbers, reattachment and blowout. The experiments are based on CH chemiluminescence to visualize the flame structure and particle image velocimetry to investigate the flow field around the lifted flame stabilization zone.

The stable lifted jet methane flames at Re=4800 show that the flame base is broad with intense emissions, indicating relatively high reaction rates. At high Re numbers of 6400 and 8300, CH* distribution shapes at the flame bases appear more irregular and some flame islands or flame holes are generated. This shifts reflects that the flame base tends to become unstable as the Re number increases. In the images of the entire flames we observed high CH* density thick, stretched flame bases and low CH* density dimmed flames downstream, which reflected the obvious gradients in flame zones. This verified that the lifted flames get maximum heat release at the flame bases and the heat release decreases downstream as flames propagate, which is consistent with the characteristics of a triple flame. The highest CH* concentration values at flame bases are almost constant in the three stable lifted jet flames. This indicates that stable lifted jet flame bases have the same combustion intensity. It is widely recognized from fundamental combustion theory that premixed flames (the expected combustion mode at the leading edge) tend to have higher reaction and heat release intensities than diffusion flames at the same fuel and oxidizer mixture conditions. The visualized characteristics of flame bases are typically partially premixed and very similar to
an original triple flame. Neither a single diffusion flame nor a stoichiometric premixed flame alone can achieve this.

The analysis about flame holes in the three Re numbers proves that flame holes act against the flame stability. Flame holes are generated closer to the flame base as the flow rate increases. In addition, flame holes appear more and tear the flame base more severely. They are more prevalent at high Re numbers, weakening the flame’s stability. Although flames holes have been visualized in our research group, the present results offer some useful information about the structure and dynamics of the flame holes due to the choice of the visualization method and the inlet conditions.

During the flame reattachment, locally high CH* intensity zones in the flame base stabilize the flame. Also, the locally high CH* intensity zones disappear as the flame base approaches the burner rim. This trend is expected since flame attachment also involves heat losses from the flame to the burner rim. The reattachment process starts with only a few points at the flame base and the velocity gradient profile is steep. Next, more points at the flame base move upstream until all points at the flame base attach to the nozzle. Meanwhile, the velocity gradients at the flame base gradually decrease. Once the lifted flame changes to an attachment flame, the CH* distribution type changes completely. The CH* density distributes lower densities upstream and higher densities downstream, which is contrast to a lifted jet flame, but is the same as a pure laminar diffusion flame.
The flame blowout shows that the flame base also holds unstable partially premixed conditions during the procedure. As the flame base becomes even more unstable, the entire flame follows the trend. This may lead us to believe that the flame base is responsible for the whole lifted jet flame stability. The simple visualization and analysis of flame bases is not enough to determine what the lifted flame stabilization mechanism is, but it has proved that no matter what the lifted jet flame condition is (stable, reattaching or blowout), flame base shapes always look like stretched partially premixed flames, and the stability of the entire flame depends only on the stability of the flame base.

The following chapters will investigate the flame base structures using flow and chemistry characteristics. An experimental PIV method and some simulation methods are implemented. The stabilization mechanism of lifted jet flames will be discussed in detail.
Chapter 3. Leading-Edge Velocities and Lifted Methane Jet Flame Stability

In contrast with premixed flames, diffusion flames do not have a mechanism to propagate. The lack of propagation mechanism raises important questions on the mechanism of flame stabilization under lifted flame conditions, since these flames have to counter the inlet flow and turbulence conditions. Images of flame position and flowfield morphology are presented from flame chemiluminescence and particle image velocimetry (PIV) measurements. In the present study, PIV experiments were carried out to measure the methane jet lifted-flame flowfield velocities in the vicinity of the flame leading edge. Specifically, velocity fields within the high-temperature zone were examined in detail, which complements previous studies, whose prime focus is the flowfield upstream of the high temperature boundary. PIV data is used not only to determine the velocities, but along with chemiluminescence images, to also indicate the approximate location of the reaction zone (further supported by the through the computed leading-edge flame velocity distributions). The velocity results indirectly support the concept that the flame is anchored primarily through the mechanism of partially premixed flame propagation.
3.1 Introduction

The stabilization mechanisms of turbulent jet lifted flames have long been the topic of combustion research and the major studies have been reviewed (Pitts, 1988 and Lyons, 2007). The premixed flame theory, the scalar dissipation rate theory, the turbulence intensity theory, large eddy dissipation theory and edge flame concept are typical theories employed.

The premixed flame theory implies that the flame base is fully premixed and at stoichiometric condition by Wohl et al. (1949), Vanquickenborne et al. (1966) and Burgess et al. (1999). However, studies by Kelman et al. (1998), Schefer et al. (1998) and Watson et al. (2003) show fuel-air mixture upstream of the flame is subject to significant turbulent fluctuation and cannot be classified as only fully premixed. The scalar dissipation rate theory claims that the extinction of diffusion flamelets controls jet lifted flame stabilization and flame base stabilizes where the scalar dissipation rate is below a critical value (Peters, 1983). However, studies have shown that the scalar dissipation rates do not reach levels thought to cause extinction of the leading edge based on comparison with extinction data for counter diffusion flames (Watson et al., 2003). The turbulence intensity theory argues that turbulence intensity at the base controls the flame speed (Kalghatgi, 1984). Some studies indicate the lifted flame base is located at a radial location that is far from the centerline, where turbulence intensities are small (Upatnieks et al., 2004). The large eddy dissipation theory (Miake-Lye et al., 1988; Demare et al., 2001), which is involved in many global theories, such as auto ignition, large eddy structures, and scalar dissipation rate theory, needs more investigation. The edge flame concept (Upatnieks et al., 2004; Buckmaster, 2002), consistent
with triple flame structures, assumes the flame leading edge can propagate upstream to counter the local flow field and stabilize the flame.

From the studies on lifted jet flame stabilization so far, the current understanding is that a partially-premixed type of edge flame may be a successful emerging model. Given that a prime importance of experimental data is to lead model development, one of the important parameters to be assessed is the velocity field at the lifted-flame base edge. Many new experimental research efforts have been performed in recent years, due in part to developments in optical techniques, such as particle image velocimetry (PIV). Advances in PIV are particularly beneficial for jet flame studies since they provide a two-dimensional planar measurement of velocity, which can produce plane axial velocities conditioned on instantaneous reaction-zone leading-edge position. One such study by Muñiz and Mungal (1997) involved the application of PIV to a lifted methane jet flame over the range of Re from 3800 to 22,000. Supported by their results, they argued that the reaction zone seeks out relatively low velocity regions of the flow field and that the flame propagates to fulfill the criterion of flame propagation counterbalancing the incoming flow of reactants. This study also examined the reaction zone for evidence of triple flame like behavior at the flame’s leading edge (Ruetsch et al., 1995). Mansour et al. (2006) also argued that for the existence of triple flames structures using species concentration images.

Watson et al. (1999) sought to identify edge flame structures in lifted flames explicitly, using CH fluorescence to infer the reaction zone location. The distortion of the edge flame structure noted by Veynante et al. (1994), however, makes direct identification of
the various branches difficult in turbulent flames, and controversy still exists as to the regimes for their existence.

Su et al. (2006) argued that statistics of the fuel mole fraction at the instantaneous high-temperature interface show that the flame stabilization point does not generally correspond to the most upstream point on the interface (called here the *leading point*), because the mixture there is typically too lean to support combustion. Instead, and they contended that the flame stabilization point lies closer to the jet centerline relative to the leading point. Conditional axial velocity statistics indicated that the mean axial velocity at the flame front is ≈ 1.8 \( S_L \) where \( S_L \) is the stoichiometric laminar flame speed. The PIV seeding used was a glycerol–water fog, which evaporates at elevated temperatures. The flame base edge was not as accurately indicated at the high temperature interface by this technique (as with tracking combustion intermediates) and it is possible that the predicted position of the flame base was impacted by such inaccuracies.

Some researchers who support edge flames theory such as Upatnieks et al. (2004) maintained that two propagation velocities of the edge flame are important. One is the actual burning velocity of the flame relative to the disturbed flow, which is of the order of the laminar burning velocity. The second is the effective propagation velocity of the whole edge flame. It is in this spirit of examining the bulk flame motion into the reactants in the laboratory frame that the following research is reported.

The objectives of this investigation are to use the methane jet flame
chemiluminescence images and raw PIV data to determine the flame position and flame edges. As opposed to previous studies, which tend to examine velocities upstream of the reaction zone, the present study focuses on velocities crossing into the high temperature zone. In this approach, the velocity field in the vicinity of the upstream portion of the reaction zone is examined in detail, along with flow behavior in the surrounding regions. Given the state of the field, these velocity fields are examined for elements that support the existence of premixed branches (i.e., flow steering across (partial) anchor-shaped reaction zones). The velocities found are compared to the laminar averaged premixed flame speeds and the variation of the velocities through the reaction zone is investigated. While studies of reactive scalars at the leading edge yield unclear results as to the morphology of the various flame branches, the details of the velocity jumps inside the high temperature zone are quite consistent with those of a partially premixed flame region. Thus, a contribution of this paper is in the area of supporting partially premixed combustion through velocity field data, rather than through arguments based on reactive-scalar field data.

3.2 Experimental Set-Up

The experiments were carried out at the Applied Energy Research Laboratory of North Carolina State University. The schematic representation of the experimental setup for the simultaneous particle image velocimetry (PIV) measurements is shown in Figure 3.1(a). The jet flame burner is a stainless steel pipe nozzle with an inner diameter of 3.5 millimeters (mm) and a length of 50 centimeters (cm) for a fully developed flow. The schematic of burner is shown in Figure 3.1(b). The apparatus is installed vertically and provides a top-hat
velocity at the nozzle’s exit and delivers 99% pure methane. A cylindrical tank filled with the 0.5-micrometer (μm) silica is connected with the methane fuel source and burner pipe to achieve seeding. The PIV system consists of two Nd:YAG laser, a dye laser, a digital high-speed camera (resolution with 1008 × 1018) and various optics (labeled as numbers of 1-11). The two lasers are built on a single compact platform (Continuum Minilite™ PIV), providing a symmetrical output beam at 532 nanometers (nm). It consists of the two pulses with equivalent beam uniformity and polarization, each at energy of 25 milli-joules (mJ). The time separation between the two pulses can be set to as low as 10 nanoseconds (ns). The trigger, connected to the lasers and the high speed camera, can activate the laser and camera simultaneously.

The flow parameters examined are at a jet exit velocity as 22.6m/s, giving a Reynolds number $Re = \frac{uD}{\nu} = 4794$ without co-flow. Here, $u$ is the jet exit velocity, $D$ presents jet diameter and $\nu$ presents kinematic viscosity at the cold fuel conditions, respectively. The lift off height achieved is approximately 3.1 cm. The laser sheet covers the full extent of the flame leading-edge.
Figure 3.1 (a) Schematic of PIV experimental arrangement and (b) Schematic of burner.
All the images are in the same coordinate system with the 76 mm × 77 mm field of view centered at 38 mm downstream (10.86 nozzle diameters). The raw PIV data is examined and processed using PIVlab 2000 software (Han and Mungal et al., 2000) in an iterative processing technique proposed by Westerweel (1997). It went through seven iterations with decreasing offset as the displacement calculations converged. The final window size was limited to 64 × 64 pixels with 50% overlap. Each PIV image resolution is slightly different because of changes in the spacing ranges of the flame images. The resolutions range from 0.5~1.2 vectors/mm.

3.3 Results and Discussions

A critical component of understanding the structure and dynamics of the stabilization region of a lifted flame is to investigate the flow patterns around the leading edge of the flame. Triple flame theory proposes a number of characteristics of the flow around the triple flame (the leading edge trailed by the diffusion flame). Important aspects of this characteristic are the presence of flow lateral divergence ahead of the flame and its subsequent convergence behind the flame. This divergence is closely associated with the presence of the lean and rich branches in the triple flame. The initial divergence results in an initial deceleration of the flow ahead of the flame to values comparable to the laminar flame speed. Therefore, triple flames can sustain higher incoming speeds (prior to the flow divergence) than their corresponding planar flames. Ruetsch et al. (1995) analysis suggests that the ratio of the incoming speed to the laminar flame speed is of the order of the square-root of the density ratio across the flame; and therefore, it is greater than unity. Figure 3.2(a)
shows the streamlines for triple flames with small and large mixing thicknesses based on the DNS simulations of Ruetsch et al. (1995). These authors superimposed the two streamline patterns to determine how the flow redirection differs in these two cases. Both of the situations have similar morphologies (with divergences near the triple flame edge from both lean and rich sides), which is one of triple flames characteristics, yet the flame structure width, associated with a prescribed width of the scalar mixing layer, is quite different; yet the effect of the width on the streamline divergence is minimal. This concept prompted the study to examine the velocity fields in detail, rather than proceed with further high resolution scalar measurements, and look for trends in the velocity fields and streamlines in the vicinity of the leading edge. Figure 3.2(b) shows the schematic of a similar laminar triple flame propagating into a fuel concentration gradient. The flame structure is indicated by iso-contour lines of the reaction rate. The bottom graph shows profiles of the horizontal velocity component along stoichiometric line for a propagating triple flame (-) and a planar premixed flame (- - -) from Ruetsch et al. (1995)). At the triple flame points, the flame speed is the same as the premixed, and in the flame zone, downstream next to the triple flame point, the flame speed is approximately 2.4 times the triple flame point speed (2.4 times the laminar flame speed). Also shown is the pure premixed flame assumption downstream, with a constant 4 times the premixed laminar flame speed.
In this study, high temperature zones are determined using the following strategy: for every flame image, the domain with considerable flame fluorescence is examined (i.e., bright luminescent background (as opposed to bright particles)). In addition, in bright zones, high temperature zones (with low density seeded particles) grayscales are more uniform locally than non-flame zones (with high density seeded particles). Therefore, in bright zones, the gradients of grayscales in flame zones are much smaller than non-flame zones. Thus, we

Figure 3.2 (a) Streamlines for triple flames with small and large mixing thicknesses (from Ruestch et al., 1995) and (b) Contour lines of the reaction rate along with the horizontal velocity component at the stoichiometric or symmetry line for a stabilized triple flame (-) and planar premixed flame (...) (from Ruestch et al., 1995).
have estimations of regions of chemical reaction using the seed particles as well as chemiluminescence magnitudes. The locations of high temperature zones are estimated empirically using the second derivative magnitudes of image grayscales less than 2. Figure 3.3(a) is a series of the experimental image results (including 6 cases from case 1 to case 6) and shows the red zones as the proposed high temperature zones.

Compared to other studies of jet flames with seeded co-flow, the study of free jet flames in the present paper focuses only on the hot zone. Inside the determined flame zones, in the vicinity of the large velocity gradients near the flame-base edge, two groups of points are selected. One group (called group 2, covered by a polygon box) contains abutting lower velocity points, which are at the flame edge. The other group (called group 1, located higher than the polygon box, but sometimes somewhat overlapping) is made up of abutting high velocities points, which are next to the flame edge downstream portion. Not all polygon boxes of left and right flame edges are labeled for each case because sometimes the vector field cannot cover the whole flame edges or noises there are too big. Further downstream, the magnitudes of velocities are even larger than group 1 that indicates the flame propagating downstream. The higher velocity group points are generally downstream of the lower velocity group. The points at the lowest y position, in the low speed group, are considered as the flame base edge velocity \( v_2 \). In the high speed group, the points downstream abutting against the flame edge are considered as \( v_1 \). Thus, \( v_1, v_2 \) and the ratio of \( v_1/v_2 \) could be examined as the characteristics of the reaction-zone edge inside the hot zone and are listed in Table 3.1. Subject to a temperature gradient, particles experience a force (thermophoresis) in
the direction opposite to that of the temperature gradient. This results in a flame thermal layer slightly thicker than the actual one and the flame front could move to the region of expanding gases. For particle diameter of $d_p = 3 \, \mu m$, research has shown velocity measurement uncertainty with thermophoretic effect is of the order of cm/s and less than 3 cm/s using the velocity lag profile from Stella et al. (2001). In addition, it decreases with decreasing particle diameter. For seeding particles with a diameter of 0.5 μm in our experiments, the maximum uncertainty does not exceed 2 cm/s. At flame base, our measured velocity data is larger than either 1.16 m/s (116 cm/s) for group 1 or 0.45 m/s (45 cm/s) for group 2 that has a much bigger magnitude than the uncertainty. Therefore, thermophoresis does bring some errors into the measuring velocity field, but the magnitudes are small.
Figure 3.3 (a) High temperature zones and flame edges (polygons).
Eddies are shown in Figure 3.3(b) using vorticities. There are sometimes large eddies near flame edges (bases on large vorticity values) such as case 3 and the left flame edge in case 4. Figure 4 to figure 9 are corresponding results of 6 cases of Figure 3.3 which include the methane flame jet fluorescence and PIV images, streamlines passing through flame edges and the velocities fields calculated at their left or right lifted flame edges. Figure

**Figure 3.3** (b) Flame edges (polygons) and vorticity distribution.
3.4 to Figure 3.9 show some eddies from streamline method directly, which just have small intensities or very lower magnitudes compared to those of Figure 3.3(b). The “a” and “b” series of Figure 4 to figure 9 represent streamlines (constructed by connecting the tangent lines of the velocity vectors) passing through the polygon flame edges. All the magnitudes of velocities of points used to calculate the $v_1$s and $v_2$s are labeled directly in either the “c” or “d” series of figures. In addition, flame edge locations are indicated by oval circles. Since the vector field intensity is much lower than streamlines, the streamlines may not be continued at every point, and they could be overlapped at some locations (3-D). Also, the velocity magnitudes are reported in the datasets and important velocities are given on the figures.

Case 1, 3, and 5 show three different relative positions between the flame base and eddy in the vicinity of the base. In case 1, the eddy is just higher than flame edge, while an eddy located just lower than the flame edge in case 3 and an eddy position much lower than the flame edge is shown in case 5. These observations support the notion that flame edge positions have no special relationship with the presence of an eddy.

Both cases 2 and 4 have no obvious eddies near the flame base. These streamline distributions near flame edges are the most common situations witnessed in our experiments. However, case 2 has a streamline divergence toward both fuel and air sides ; case 4 streamlines only diverge toward one side, either the air side (case 4, flame left edge) or the fuel side (case 4, flame right edge).
The streamline distributions in case 6 are rarely witnessed in the experimental results. Because of the eddy slow rotational speeds, the spiral motion focuses as singular points are easily captured by streamlines. The eddy morphology of case 6 at the left or right flame edge is also different. The left edge’s eddy only twists toward downstream directions (with a 90° range), while the right one twists in all directions (with a 360° range).

The six cases represent the general characteristics of the streamline and interrelated eddy styles near flame edges. In figures 4 through 9, dashed arrow straight lines indicate the streamline divergence directions, dashed circles label the eddy positions, and dashed triangles probe the singular points.

Figure 3.4 series are the results of methane jet flame image of case 1. The rectangular box is supposed to include the flame edge because of the large velocity gradient and streamlines divergence in that region. The velocity of point 4-c3, 1.34 m/s, is largest in the rectangle. The other five points 4-c1, 4-c2, 4-c4, 4-c5 and 4-c6 have much smaller velocities, and the points 4-c2 and 4-c6 are abutting against point 4-c3. So the \( v_2 \), for this figure, is the average of points 4-c2 and 4-c6, which is 0.63 m/s, and the \( v_1 \), considered at point 4-c3, is 1.34 m/s. This is consistent with the morphology of the chemiluminescence zone and the jump in velocity being approximately 2, representing the flow into the premixed edge of the reaction zone.

Figure 3.5 series show the results of methane jet flame image of case 2. The flame edges are contained in the polygons (in Figure 3.5(c)) and in figure 3.5(d)). The \( v_2 \) in figure
3.5(c) is 0.7 m/s, which is the average of points 5-c1 & 5-c3, and the $v_1$ is the value of 5-c2, 1.7 m/s. In Figure 3.5(d), the $v_2$, 0.64 m/s, is the average of the three points in the top line of the rectangle, and the $v_1$ is the average of 5-d1 and 5-d2 which is 1.375 m/s. At this right flame edge, air is seen to be strongly entrained.

Figure 3.6 series are the results of methane jet flame image of case 3. Figure 3.6(a) shows there is a large eddy nearby the left flame edge, where air is coming in to the flame edge significantly. The $v_2$, 0.737 m/s, is the average of the three points of 6-c4, 6-c5 and 6-c6 in the rectangle, while the $v_1$ is 1.767 m/s, which is the average of points 6-c1, 6-c2 and 6-c3.

Figure 3.7 series show both left (Figure 3.7(c)) and right (Figure 3.7(d)) flame edges of case 4. At the left flame edge, the $v_2$ is the average of points 7-c1, 7-c4 and 7-c5, which is 0.64 m/s, and the $v_1$ is 1.66 m/s, the average of points 7-c2, 7-c3 and 7-c6. At the right flame edge, the $v_2$ is the average of points 7-d3 and 7-d4, which is 0.695 m/s, while the $v_1$ is 1.685 m/s, the average of points 7-d1 and 7-d2. Figure 8 series (of case 5) are the fifth results. Figure 3.8(c) shows the left flame edge with the $v_2$ as the average of the upper line points in the rectangle, which is 0.45 m/s, and the $v_1$, the average of 8-c1, 8-c2 and 8-c3, is 1.16 m/s. The streamlines at the left flame edge indicates flow towards the surrounding air, which is significant.

In Figure 3.9 (of case 6), at the left flame edge in figure 3.9(c), the $v_2$ is 0.55 m/s which is calculated by the average of points 9-c4, 9-c5 and 9-c6, while the $v_1$ is 1.41 m/s, the average of points 9-c1, 9-c2 and 9-c3. At the right flame edge in figure 3.9(d), the $v_2$ is set as
the average of point 9-d4, 9-d5 and 9-d6 which has the value of 0.53m/s, and the $v_1$ is 1.34m/s, set as the average of points 9-d1 and 9-d2. The right flame edge has what appears to be a large scale vertical structure at the jet edge.
Figure 3.4 Streamlines passing through the flame edge and velocity variations in case 1.

(a) Streamlines passing through the flame edge of case 1. (c) Velocity variation at the flame edge of case 1. The velocities in the rectangle are 0.28 m/s, 0.62 m/s, 1.34 m/s, 0.35 m/s, 0.5 m/s, 0.64 m/s. (ordered by left to right and top down)
Figure 3.5 Streamlines passing through the flame edge and velocity variations in case 2. Streamlines passing through the left (a) and right (b) flame edges of case 2. (c) Velocity variation at the left flame edge of case 2. The points’ velocities in the polygon are 0.42m/s, 0.8m/s, 0.56m/s, 0.56m/s and 0.84m/s (ordered by left to right and top down). The velocity of point 5-c2 is 1.7m/s. (d) Velocity variation at the right flame edge of case 2. The six points’ velocities in the rectangle are 0.65m/s, 0.79m/s, 0.49m/s, 0.21m/s, 0.2m/s, 0.07m/s (ordered by left to right, top down). The velocities of points 5-d1 and 5-d2 are 1.4m/s and 1.35m/s.
Figure 3.6 Streamlines passing through the flame edge and velocity variations in case 3.

(a) Streamlines passing through the flame edge of case 3. (c) Velocity variation at the flame edge of case 3. The velocities of the six points in the rectangle are 1.06m/s, 0.81m/s, 0.92m/s, 0.7m/s, 0.81m/s and 0.7m/s (ordered by left to right, top down). The velocities of the three points of 6-c1, 6-c2 and 6-c3 are 1.63m/s, 1.82m/s and 1.85m/s.
Figure 3.7 Streamlines passing through the flame edge and velocity variations in case 4.

(c) Velocity variation at the left flame edge of case 4. The points’ velocities in the polygon are 0.85m/s, 2.06m/s, 1.77m/s, 0.39m/s, 0.69m/s, 1.15m/s (ordered by left to right, top down).

(d) Velocity variation at the right flame edge of case 4. The points’ velocities in the polygon are 0.93m/s, 0.66m/s, 0.46m/s, 0.42m/s, 0.45m/s (ordered by left to right, top down). The velocities of points 7-d1 and 7-d2 are 1.8m/s and 1.57m/s respectively.
(a) Streamlines passing through the left flame edge of case 5. (c) Velocity variations at the flame edge of case 5. The points’ velocities in the rectangle are 0.7 m/s, 0.34 m/s, 0.30 m/s, 0.45 m/s, 0.71 m/s, 0.99 m/s, 1.0 m/s and 0.8 m/s (ordered by left to right, top down). The velocities of 8-c1, 8-c2 and 8-c3 points are 1.02 m/s, 1.25 m/s and 1.21 m/s.

Figure 3.8 Streamlines passing through the flame edge and velocity variations in case 5.
Figure 3.9 Streamlines passing through the flame edge and velocity variations in case 6.
(c) The points’ velocities in the polygon are 0.76m/s, 0.47m/s, 0.17m/s, 0.44m/s, 0.54m/s, 0.73m/s. The velocities of 9-c1, 9-c2 and 9-c3 are 1.55m/s, 1.32m/s and 1.36m/s. (d) The points’ velocities in the polygon speeds are 0.66m/s, 0.37m/s, 0.32m/s, 0.41m/s, 0.6m/s, 0.54m/s, 0.53m/s, 0.69m/s, 0.33m/s and 0.23m/s (ordered by left to right, top down). The velocities of points 9-d1, 9-d2 and 9-d3 are 1.31m/s, 1.37m/s and 1.51m/s.
Analyzing the selected data, the streamlines in figure 3.4 through figure 3.9 are compared near the flame edges with the streamlines of a triple flame in figure 3.2. In the current experimental results, the streamlines into the reaction zones have similar trends and divergences, as one would expect from a triple flame and laminar lifted flame (Lee et al., 1997) structures. Virtually all of trends in figures 3.4 to 3.9 show that the streamlines evolve to near straight parallel lines above the initial divergences positions, similar to what is witnessed in the triple flame simulations. Figure 3.5(a) & (b) streamlines diverge toward the two sides (both fuel and air). While the results of Figures 3.4(a), 3.6(a), 3.7(a), 3.8(a), 3.9(a) and 3.9(b) show similar divergences to air side. The other result of figure 3.7(b) shows streamlines directed toward to fuel side. In addition, the present study finds that the eddies near the flame edge, such as Figures 3.4(a), 3.6(a), 3.8(a), 3.9(a) and 3.9(b) flow fields, are similar to those seen in Kelman et al. (1998).

All of these cases show that air is entrained into the reaction zone regardless of the existence of a large eddy near flame edge. It was also shown by Domingo and Vervisch (2008) that a triple flame is able to survive strong interaction with vortices by adjusting its structure to a new transient environment. In addition, no evidence supports this flame edge with the large eddy is one sequence of flame edge evolutions since only one large eddy at most could be found near flame edge. There is no evidence to indicate that the flame edges must be located at a fixed vortex position, such as the second or third vortex starting from jet inlet. It only offers that flame edge may stretch and has no the whole triple flame shape. The fuel lean, fuel rich and diffusion tri-brachial structure (triple flame) at the flame edge may
lose one or two premixed branches and merge into the trailing diffusion flame, which has been examined in previous studies and is still an area of contention.

Ruetsch et al. (1995) performed a theoretical and computational study of triple flames, results of which are shown in figure 3.2(b). For small cross-stream gradients in mixture fraction, the flame propagation speed is \( u_F \approx S_L \sqrt{\rho_u / \rho_d} \), where \( u_F \) is the flame speed relative to the flow well upstream, \( S_L \) is the stoichiometric laminar flame speed, and \( \rho_u \) and \( \rho_d \) are the densities far upstream and far downstream of the flame. For an upstream stoichiometric methane–air mixture at 298 K, where the downstream mixture consists of combustion products at 2210 K, \( u_F \approx 2.4 S_L \). The flame inflow axial velocities measured by Muñiz and Mungal (1997) and by Han and Mungal (2000) were typically less than 3\( S_L \).

In the present experiments, velocity magnitudes of the flame base edge range from 0.45~0.737 m/s and the \( v_1 \)s, which is the next to the flame edge velocities, range from 1.16 to 1.767 m/s. These generally agree with the heat release effect proposed by Boulanger et al. (2003). They support the notion that in lifted jet flames, the effect of the heat release causes the deflection of the flow upstream of the curved front, which has the net result of making the reaction propagate faster than \( S_L \), the propagation speed of a fully premixed and planar stoichiometric flame. This flow deflection also induces a decrease of the mixture fraction gradient in the trailing diffusion flame. The velocity of the overall reaction zone structure is therefore greater than the premixed burning velocity.
A summary of the aforementioned discussion, however varied, results in the identification of a trend through the data shown in table 1. Most results (Table 3.1) indicate that the local velocities are larger than 0.4 m/s. This also agrees with Upatnieks et al. (2004), which found the effective propagation velocity of the entire edge flame with respect to the upstream (undisturbed) flow exceeds the laminar burning velocity. Ghosal et al. (2001) introduced a heat release effect parameter $\alpha = (T_s - T_0)/T_s$ where $T_0$ is the temperature of the fresh gases and $T_s$ is the adiabatic temperature of a stoichiometric flame. In typical hydrocarbon flames, $\alpha$ is 0.8, and the flow speed at the base of the lifted flame (equal to the triple flame speed) is almost twice the adiabatic flame speed for the corresponding stoichiometric mixture. In the present results, the flame edge speed $v_2$ is larger than laminar flame speed, but less than twice of the laminar speed. Chung (2006) showed the laminar flame edge has different velocities at transition (larger than $S_L$), tri-brachial (close to $S_L$), bi-brachial (smaller than $S_L$, sometimes negative) and mono-brachial (negative close to extinction), however, our results only showed the velocities are larger than $S_L$ and there are no clues about the bi-brachial and mono-brachial phenomena.

In addition, shown in table 1, the average ratio, of velocity magnitudes at the flame base edge, is approximately 2.42 (ranged from 2.13 to 2.59), which is rather close to that of a typical triple flame, of 2.4, than a planar premixed flame, of 4. This agrees with the flame-edge concept supported by Upatnieks et al. (2004) and their data also show no significant correlation between propagation speed and the passage of large eddies.
Table 3.1: Velocity magnitudes and ratios at flame edges.

<table>
<thead>
<tr>
<th>Figure #</th>
<th>Velocity of downstream next to flame edge : $v_1$(m/s)</th>
<th>Velocity of flame edge upstream: $v_2$(m/s)</th>
<th>Ratio of $v_1/v_2$</th>
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<td>4(c)</td>
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<td>0.63</td>
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<td>1.7</td>
<td>0.7</td>
<td>2.43</td>
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<td>1.767</td>
<td>0.737</td>
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<td>7(c)</td>
<td>1.66</td>
<td>0.64</td>
<td>2.59</td>
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<tr>
<td>7(d)</td>
<td>1.685</td>
<td>0.695</td>
<td>2.42</td>
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<td>1.16</td>
<td>0.45</td>
<td>2.58</td>
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<td>0.55</td>
<td>2.56</td>
</tr>
<tr>
<td>9(d)</td>
<td>1.34</td>
<td>0.53</td>
<td>2.53</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td><strong>1.49</strong></td>
<td><strong>0.62</strong></td>
<td><strong>2.42</strong></td>
</tr>
</tbody>
</table>

3.4 Conclusions

Experimental PIV measurements and flame chemiluminescence imaging identify the flow patterns at the flame leading edge and compares the observations to flow conditions from triple flame theory. The data presented shows the presence of a velocity field consistent with that of a partially premixed edge-flame.

The flame edges (next to the polygons in the flame images) reveal that the streamlines have similar divergence characteristics to edge flames. Above the flame edge location, the streamlines downstream have nearly straight parallel arrangements, which are also similar to
that modeled as triple flames in numerical studies. The divergences can be located in large eddies, but are not in some cases, and still indicate fuel and air mixed at the flame edge. This is similar to the claim by Upatnieks (2004) that the flame base does not need to be in contact with eddies to remain anchored at one fixed location, and the large eddies could be just an ancillary factor in flame base oscillation. However, the detailed flame edge structure is still not clearly rendered; it might be tri-brachial, bi-brachial or mono-brachial and the mass fractions gradients are not obtained in the present experiments - the edge flame propagation speed measured supports the flame edge detailed structures. (Chung S.H., 2008). Therefore, in this Re case, the lift-off jet flame stability is argued to be driven by a partially-premixed flame mechanism.

The propagation velocities at the flame edge are, in general, higher than that of the corresponding laminar triple flames. The flame edge speed \( v_2 \) is larger than laminar speed \( S_L \) (0.4m/s), and the \( v_1 \) downstream next to the flame edge is larger than 0.96 m/s which is approximately \( 2.4S_L \).

Using relatively primitive particle tracking/PIV and chemiluminescence techniques, meaningful facets of the reaction zone can be extracted, as evidenced from the results summarized in table 3.1. This approach shows promise for utilization in interpreting cinema PIV studies of reaction zones.
Chapter 4. DNS Investigation of an Unsteady Shear Layer Lifted Hydrogen-Air Flame

4.1 Introduction

Fundamental knowledge of the lifted flame stabilizing mechanism will lead to the development of predictive models used in engineering CFD for the design and optimization of fuel efficient, clean burning combustion devices. Many studies and theories involving both experiments and simulations have been proposed. Chapters 3 provided experimental evidence in support of the triple flame theory as a viable theory for lifted jet flame stability. In this chapter, we used a DNS simulation method to investigate the flame edge structures.

The rapid growth in computational capabilities has presented both opportunities and challenges for DNS of turbulent combustion. In DNS, the instantaneous governing equations are solved without averaging or filtering; therefore, all relevant continuum scales are resolved on the grid without any turbulence closure models using accurate high-order numerical methods for computational efficiency. Such simulations are costly, requiring many CPU hours on parallel computers, up to several billion grid points, and generating tens of gigabytes of data. The code used in this chapter is called S3D which is a massively parallel DNS solver developed at Sandia National Laboratories (2005). S3D solves the full
compressible Navier–Stokes, total energy, species and mass continuity equations coupled with detailed or simplified chemistry. So considering the S3D running cost, we only simulated an unsteady shear layer flame using S3D. Shear layer flames are similar to but simpler than jet flames. The DNS study attempts to identify the role of chemistry on flame structure and stabilization mechanism using a global four-step mechanism for hydrogen chemistry. Chapter 4 looks more closely at the role of fluid dynamics with simple chemistry within the more realistic configuration of a lifted jet diffusion flame.

In chapter 3, streamline divergence at flame edges was used to investigate the flame base location and flow characteristics at flame edges. This method is extended in this chapter on the unsteady shear layer flames. Also, flame structures are investigated and density weight displacement flame speed $S_d^*$ is calculated. The streamline divergence at flame edges and the normalized flame index (N.F.I) clearly show flame bases with a full triple flame shape and flame bases always moving together. Therefore, triple or edge flames stabilize the lifted turbulent flames.

4.2 Formulation and Numerical Implementation

4.2.1 Governing equations in S3D

The DNS code solves the Navier–Stokes, species, and energy conservation equations for a compressible reacting gas mixture. The numerical scheme employs an eighth-order centered finite difference stencil for spatial differencing and explicit fourth-order six-stage low-storage Runge–Kutta method for time advancement. Neglecting body force, the mass
transfer through temperature gradient (Soret effect) and energy transport through concentration gradients (Dufour effect), the governing equations are written as

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \quad (4-1)
\]

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j + \delta_{ij} \rho - \tau_{ij}) = 0 \quad (4-2)
\]

\[
\frac{\partial (\rho e_t)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j e_t + u_j \rho + q_j - u_i \tau_{ij}) = 0 \quad (4-3)
\]

\[
\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j Y_k + \rho Y_k V_{kj}) - W_k \omega_k = 0 \quad (4-4)
\]

where \( Y_k \) is the mass fraction of species \( k \), \( W_k \) is the molecular weight of species \( k \), \( \tau_{ij} \) is the stress tensor given by \( \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \). \( q_j \) is the heat flux vector given by \( q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{n} h_k V_{kj} \). \( V_{kj} \) is the species mass diffusion velocity along the \( x_j \) direction, \( \omega_k \) is the molar production rate of species \( k \). \( e_t \) is the specific total energy (internal energy plus kinetic energy), \( e_t = \frac{u_i u_j}{2} - \frac{p}{\rho} + h \). \( h \) is the total enthalpy (sensible plus chemical). Relevant thermodynamic relationships between enthalpy and temperature for an ideal gas mixture is \( h = \sum_{k=1}^{n} Y_k h_k \), \( h_k = h_k^0 + \int_{T_0}^{T} C_{p,k} dT \). Assuming an ideal gas mixture, the equation of state is given as \( p = \frac{\rho R_u T}{W} \). Where \( R_u \) is the universal gas constant and \( W \) is the mixture molecular weight given by \( \frac{1}{\left( \sum_{k=1}^{n} \frac{1}{W_k} \right)} = \sum_{k=1}^{n} X_k W_k \).
4.2.2 Computation domain settings

A modified version of the Navier–Stokes characteristic boundary condition treatment is applied. Boundary conditions are inlet at the inlet boundary of $x =0$ and nonreflecting in the other directions which means any characteristic waves with a net component leaving the domain are allowed to exit the domain, while no disturbances from outside the domain are allowed to enter it.

The flame structures and stability in unsteady lifted combustion zones have been simulated with hydrogen ($H_2$) air 4-step chemistry in a 2D turbulent shear layer reaction flow using DNS (Direct Numerical Simulation). These governing equations were outlined in section 4.2.1. The governing equations are supplemented with additional constitutive relationships, such as the ideal gas equation of state, and models for reaction rates, molecular transport and thermodynamic properties.

The DNS simulation was performed in a square region of 2.25 cm ×2.25 cm with uniform meshes. Both fuel ($H_2$ and $N_2$ with the mole ratio of 1/1.6) and air have inlet velocities of 1.5m/s, and they each occupy half (1.125cm) of the inlet boundary. OPPDIF is used to generate an initial steady laminar flame. Initially the temperature is set to 298 K and the pressure is 1 Atm. The initial flame structures as represented by temperature and species mass fraction distributions are shown in Figure 4.1. The initial lift off height of the shear layer flame is 0.5cm and there are no products below it.
The present chemical mechanism consists of 7 chemical species and 4 reaction steps. The transported chemical species are \( \text{H}_2, \text{O}_2, \text{H}_2\text{O}, \text{H}, \text{O}, \text{OH}, \text{and N}_2 \). The species mass diffusion is determined by prescribing the Lewis numbers of individual species. Lewis numbers are determined from a best fit to the mixture-averaged transport coefficients recommended for the GRI3.0 mechanism in the laminar flame and are given in Table 1. The turbulence is setting as homogenous and \( \frac{u'}{u} = 0.1 \).

**Table 4.1:** Lewis numbers of the 7 species in the \( \text{H}_2 \) and \( \text{O}_2 \) 4-step mechanism

<table>
<thead>
<tr>
<th>Species</th>
<th>( \text{Le} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H}_2 )</td>
<td>0.3</td>
</tr>
<tr>
<td>( \text{O}_2 )</td>
<td>1.17</td>
</tr>
<tr>
<td>( \text{H}_2\text{O} )</td>
<td>1.03</td>
</tr>
<tr>
<td>( \text{H} )</td>
<td>0.2</td>
</tr>
<tr>
<td>( \text{O} )</td>
<td>0.74</td>
</tr>
<tr>
<td>( \text{OH} )</td>
<td>0.75</td>
</tr>
<tr>
<td>( \text{N}_2 )</td>
<td>1.44</td>
</tr>
</tbody>
</table>

### 4.2.3 Chemical mechanism

The \( \text{H}_2 \) and \( \text{O}_2 \) 4-step reduced mechanism listed blow is modified from \( \text{H}_2/\text{O}_2/\text{NO}_x \) 5-step mechanism by Chen (1995).

\[
\begin{align*}
\text{O}_2 + \text{H} &= \text{OH} + \text{O} \quad (R_1) \\
\text{H}_2 + \text{O} &= \text{H} + \text{OH} \quad (R_2)
\end{align*}
\]
\[ H_2 + OH = H + H_2O \quad (R_3) \]
\[ H + O = OH \quad (R_4) \]

The reaction rates are originally derived by Chen et al., 1995; we neglected the NO term and modified them as follows:

\[ R_1 = \omega_1 - \omega_2 + \omega_9 - \omega_{10} - \omega_{12} - \omega_{13} \]
\[ R_2 = \omega_3 - \omega_4 - \omega_7 + \omega_8 - \omega_{12} - \omega_{13} - \omega_{14} - \omega_{22} - \omega_{23} \]
\[ R_3 = \omega_5 - \omega_6 + \omega_7 - \omega_8 + \omega_{13} + \omega_{14} + \omega_{23} \]
\[ R_4 = \omega_{11} + \omega_{12} + \omega_{13} + \omega_{14} + \omega_{22} + \omega_{23} \]

where \( \omega_1 \) to \( \omega_{23} \) are first 23 steps reaction rates in hydrogen air detailed reaction mechanism (shown in Appendix A).

### 4.3 Analysis and Discussions

The typical heat release distributions are shown in Figure 4.2. Flame edges are anchor shapes with high heat release values which may include both premixed and diffusion flame branches. Flames downstream are trailing diffusion flames with lower heat release values. Under this unsteady condition, the flame edge moving speed and detailed flame edge structure can aid us to understand the flame stability.

Figure 4.2 shows the heat release rate distributions in flames. The results at the three different times show the flame base always has the highest heat release rates and the rates
decrease sharply downstream. This obvious pattern of the heat release gradients from the flame edge upstream to downstream is also seen in the flame base visualization of CH$^*$ density from the experiments in Chapter 2. As discussed in Section 2.1, The CH method potentially brings some puny position errors if it represents heat release. However, it will not affect the overall macroscopic energy distributions on the flame base. In Figure 4.3, typical CH$^*$ distributions (Re=6400 and Re=8300) does have the same energy distribution as a triple flame or edge flame.

Also, from the heat release contours in Figure 4.2, the lean premixed branch is difficult to distinguish; whereas, because of the low flow rate and low turbulence in the simulations, the premixed rich flame branch is easy to distinguish. In the experiment of Chapter 2, the large flow rate along with the high turbulence caused the rich, branch, the lean branch, and the diffusion flame to merge downstream completely. However, this phenomenon did not increase the energy significantly in the merging region. So, it can be seen that merging did not cause a change in the energy distribution, in either the simulations (Figure 4.2) or the experiments.

Moreover, the fuel is hydrogen. Its low Lewis number (i.e. mass diffusivity) and its flammability limits may explain the non-symmetric distribution of the lean and rich branches. Although the fuel used in the simulations is different from the experimental fuel, methane. This difference should not affect conclusions about the flame edge properties.
The section develops an expression for the displacement speed $S_d$ of an isoscalar surface relative to the flow field. The analysis is based on tracking a surface on which the mass fraction $Y$, of the deficient reactant is fixed to a value in the reaction zone. The governing transport equation is:

$$\rho S_d = \rho_u S_d^* = \left[ \frac{\partial}{\partial x_j} \left( \rho D_k \frac{\partial Y_k}{\partial x_j} \right) + \omega_k \right] / |\nabla Y_k| \tag{4-5}$$

Where, $\omega_k$ is reaction rate of the species $k$ and $\rho_u$ denotes the unburnt gas density. $D_k$, the species’ mass diffusivity, is calculated as follows:

$$D_k = \frac{\lambda}{\rho C_p L_e} \tag{4-6}$$

$$\lambda = C_p A \left( \frac{T}{T_0} \right)^r ; \quad C_p = \sum C_{p,i} Y_i$$

Here, $\lambda$ is thermal conductivity, $A$ and $r$ are constants, with $A = 2.58 \times 10^{-4}$ and $r=0.4$, and $T_0 = 298K$. $V_f$, the velocity of the leading edge of triple flames moving relative to unburned gas is calculated using the following relation:

$$V_f = u - S_d^* n \tag{4-7}$$

$S_d^*$ is the magnitude of the density-weighted displacement speed and $n$ is the unit normal vector of the isocontour of $Y_k$ directed toward the unburnt gas. It is expressed in terms of the normalized local gradient vector of $Y_k : n = \frac{\nabla Y_k}{|\nabla Y_k|}$.
In order to distinguish the different flame branches, we use the normalized flame index (N.F.I) to label lean premixed, rich premixed, and diffusion flames. The N.F.I relation modified from Lock (2005) is given as

\[ N, F, I = \left[ \frac{(z - z_s)}{|z - z_s|} \cdot \frac{1}{2} \times \left( 1 + \frac{\nu_{Y_F} \nu_{Y_O}}{\nu_{Y_F} \nu_{Y_O}} \right) + 2 \right] \] (4-8)

Here, \( Y_F \) denotes the fuel mass fraction and \( Y_O \) the oxidizer mass fraction. The stoichiometric mixture fraction \( z_s \) is 0.407 in the chemistry of the simulations which lies within the diffusion reaction zone. In addition, the mixture fraction is calculated using the following Bilger formula (2005),

\[ z = \frac{0.5 (Y_{H} - Y_{H,2}) (Y_{O} - Y_{O,2})}{W_H} \frac{0.5 (Y_{H,1} - Y_{H,2}) (Y_{O,1} - Y_{O,2})}{W_O} \] (4-9)

where \( Y_H \) is the mass fraction of element \( H \), \( Y_O \) is the mass fraction of element \( O \), \( Y_{H,1} \) is the mass fraction of element \( H \) in the fuel stream, \( Y_{O,1} \) is the mass fraction of element \( O \) in the fuel stream, \( Y_{H,2} \) is the mass fraction of element \( H \) in the air stream, and \( Y_{O,2} \) is the mass fraction of element \( O \) in the air stream. The atomic weights of the elements, H and O, are \( W_H = 1.008 \) and \( W_O = 16.0 \), respectively. For different values of N.F.I, 1 means lean premixed flame branch, 2 means diffusion branch and 3 means rich premixed flame branch.

Figures 4.4, 4.5, and 4.6 show the N.F.I on the heat release rate of the unsteady flames at three different times, \( 8.39 \times 10^{-4} \) s, \( 2.10 \times 10^{-3} \) s, and \( 9.73 \times 10^{-3} \) s. Each N.F.I clearly shows the flame structures: 3 stands for rich premixed flame, 2 for diffusion flame, and 1 for
lean premixed flame. That proves that the lifted shear layer flames are triple flames. The rich premixed branch is obviously appears as a separate appendage on the diffusion flame while the lean branch is embracing it.

The b and c series of Figures 4.4 to 4.6 are streamlines passing through flame edges based on the original velocity fields, $u$ and $V_f$, respectively. Both series of streamline divergences indicate the flame edge positions. However, those based on the $V_f$ field are much more obvious and accentuated at flame edges. The density-weighted displacement speed $S_d^*$ in Figures 4.4 to 4.6 shows that the moving speed distribution is shaped like an anchor. Therefore, the entire edge of each flame is moving at a consistent speed. Also, this indicates that the lean, rich premixed, and diffusion branches could be responsible for the flame stability.
Figure 4.1 Initial flames in the shear layer turbulent flow of fuel (H$_2$ and O$_2$ molar ratio is 1:1.6) and air.
Figure 4.2 Non dimensional heat release rate, (a) at time of \(8.399 \times 10^{-4}\) s, (b) at time of \(2.10 \times 10^{-3}\) s, and (c) at time of \(9.773 \times 10^{-3}\) s.
Figure 4.3 CH$^*$ distributions in experiments at (a) Re=6400 and (b) Re=8300 (reprint Figure 2.3(b) and (c)).
Figure 4.4 (a) N.F.I. (b) Streamlines based on original velocity, and (c) Streamlines based on $V_f$ at the time of $8.399 \times 10^{-7}$ second.
Figure 4.5 (a) N.F.I, (b) Streamlines based on original velocity and (c) Streamlines based on $V_f$ at the time of $2.10 \times 10^{-3}$ second.
Figure 4.6 (a) N.F.I, (b) Streamlines based on original velocity and (c) Streamlines based on $V_t$ at the time of $9.773 \times 10^{-3}$ second.
4.4 Conclusions

The shear layer hydrogen air flame under unsteady conditions was implemented using the DNS approach with a realistic description of hydrogen chemistry. The flame structure and flow characteristics are investigated, including streamlines. From the analysis, we conclude that for the present flow conditions.

The flame structure in the shear layer turbulence flow is that of a triple flame. All three of the branches, lean, diffusion, and rich, can be identified. The structure is identified through contours of the flame index. This index is designed to distinguish burning in lean and rich premixed modes as well as burning in non-premixed mode. Another indication of the partially-premixed nature of the flame comes from the intensity of the heat release rate at the leading edge of the lifted flame compared with the trailing non-premixed flame. The results show enhanced reaction rate intensities characteristic of premixed combustion at the leading edge and consistent with the experimental observations shown in Chapter 2. The unsteady nature of the upstream flow results in a distortion of the shape of the leading edge, even though the overall triple flame structure of the leading edge is maintained.

Another indication of the partially-premixed flame structure at the leading edge of the lifted flame comes from contours of the density-weighted displacement speed. According to triple flame theory, the leading edge of the triple flame can sustain displacement speeds, which are greater than the laminar values, due primarily to the presence of lateral flow divergence ahead of the premixed branches. Though the simulation only run under unsteady
conditions, $S_{a}^*$ shows flame edge moving as a whole bulk. Also the $S_{a}^*$ distribution has an anchor shape. Streamline divergence is also a characteristic of the flame edge. The divergence may change with time and better divergence could be seen if the flame propagating effects are subtracted.

The shear layer flame simulations reflect the stabilization mechanism in lifted jet flames, but the shear layer flow simulated in this chapter has a low and uniform inlet speed on both the fuel and air sides. The flame edge developed by a shear layer flow may be qualitatively different from the one obtained in a jet flow. In hydrogen lifted jet flames, the inlet jet velocity is as high as 100 m/s while the co-flow is of the order of $10^{-1}$ m/s. As a consequence, the symmetry between the rich (inner) premixed flame branch and the lean (outer) premixed flame branch is not present. This symmetry also can be impacted by the different flammability limits for the lean and rich mixtures. Another impact effects on the extent of the premixed flame branches may be associated with the thickness of the scalar mixing layer, which can also be affected by the lift-off height (the larger the lift-off height, the longer the fuel and air streams are allowed to mix and, accordingly, the wider the scalar mixing layer is).
Chapter 5. DNS of Lifted Jet Flames at Transitional Reynolds Numbers

5.1 Introduction

In Chapter 4, we investigated the structure of a shear layer flame under unsteady conditions. Because of the inherent computational cost with detailed or reduced chemistry, the jet flame structure was not studied. In this chapter, a simpler chemistry DNS study with a general one-step chemistry is carried out. The simulations are implemented under conditions of transition to turbulence to capture the role of flow instabilities and the onset of turbulence on the flame structure and dynamics. The transitions are characterized by the onset of instabilities (e.g. Kelvin-Helmholtz Instabilities) where large-scale vortex motion dominates the mixing process (Takeno, 1994).

DNS studies have been carried out for a broad range of reacting flows (see the review of Vervisch and Poinsot 1998 and related references). However, free turbulent flows are much more difficult to simulate. First, there is no clear boundary to which the flow is confined, so the dimensions of the computational domain must be large enough to account for free-stream conditions. Second, one has to deal with spatial evolution as a result of entrainment of ambient fluid into the turbulent flow region. In view of this latter difficulty, most simulation studies of free turbulent flow have been restricted to a temporally developing flow rather than a spatially developing flow (Freund et al., 1998). Moreover,
inherent with shear-driven flows are the presence of large-scale flow structures that have to be captured along with the smallest scales associated with scalar dissipation. The topology of these large-scale structures can be inherently 2D (e.g. some Kelvin-Helmholtz instabilities) or 3D, requiring even more extensive computational resources. In the present study, we use a spatially developing turbulent round jet based on the formulation originally developed by Borsma (1998) with some modification by Miles (2010).

A typical transition flow is shown in Figure 5.1 (reprinted from Takeno, 1994). The simulation result is non-dimensional temperature contours on an attached methane air jet flame. The surrounding temperature $T_0 = 300$ K. The adiabatic flame temperature is $T_{ad} = 2225.9$ K, and the resulting non-dimensional flame temperature $\frac{T_{ad}}{T_0} = 7.419$. The flame takes a familiar configuration comprised of an upstream laminar and downstream turbulent flame. The temperature gradients are steep near the outer edges while they are quite gradual in the interior, producing thick high-temperature strips. The instantaneous distribution shows that a small-scale sinusoidal fluctuation of the fuel jet appears at the coldest temperature (blue color) on the axis, and develops into a large-scale eddy motion downstream. The outer large-scale fluctuation, on the other hand, starts downstream of the incipient point of the inner fluctuation and merges with it to produce a large-scale eddy motion along the flame surface downstream. A lifted jet flame under a transitional phase may be similar to the attached flame from Takeno (1994), but lift-off may change the flame base structure. The transitional phase is one of the many important types of lifted jet flames; and so its corresponding stability should be studied.
Since the large eddies are obvious and could be very close to the flame base or located directly on the flame base if the attached flame were to change to a lift off flame, the large eddies could play a crucial role in flame stabilization. This kind of flow condition is convenient to investigate if large eddies play a critical role in the flame stabilization. In laminar flow, there is inherently a symmetry plane that cuts through the jet axis and an axis transverse to the flow (no circumferential effects). At the onset of transition, instabilities are inherently 2D, and the presence of symmetry is still a valid observation. We denote the symmetry plane as an $x$-$y$ plane and present results primarily on these symmetry planes (2D results). However, the runs are still made in 3D.

Figure 5.1 A jet flame temperature distributions under a transition condition (Takeno, 1994).
5.2 Governing Equations

The governing equations used a low Mach number approximation as described by Najm et al. (1998). The motivation for the use of this approximation is that we are basically interested in flows with velocities which are small compared to the speed of sound. The restriction on the numerical scheme time step would be too severe if a strict solution of the full set of equations were used.

Starting from the dimensionless scale definitions as equations of 5-1:

\[ T^* = \frac{T}{T_0}, \quad t^* = \frac{t}{t_0}, \quad t_0 = \frac{L}{U}, \quad x_j^* = \frac{x_j}{L}, \quad u_j^* = \frac{u_j}{U}, \quad \mu^* = \frac{\mu}{\mu_0} \]

\[ \rho^* = \frac{\rho}{\rho_\infty}, \quad P^* = \frac{P}{\rho_\infty U^2}, \quad Re = \frac{\rho \omega UL}{\mu_0}, \quad Sc = \frac{\mu}{\rho D}, \quad Pr = \frac{C_p \mu}{k} \]  

(5-1)

The superscript of * represents a dimensionless value. The others are dimensional symbols. \( T \) stands for temperature, \( t \) for time, \( \rho \) for density, \( P \) for pressure, \( \mu \) for dynamic viscosity, \( D \) for mass diffusivity and \( k \) for thermal conductivity. \( L \) and \( U \) are the length and velocity scales. In the jet simulation, \( L \) is the diameter of the jet pipe and \( U \) is the initial jet inlet velocity.

The simplified non-dimensional low Mach number mass and momentum equations are (Borsma 1998)

\[ \frac{\partial \rho^*}{\partial t^*} + \frac{\partial}{\partial x_j^*} (\rho^* u_j^*) = 0 \]  

(5-2)

and
\[
\frac{\partial}{\partial t^*}(\rho^* u_i^* ) + \frac{\partial}{\partial x_j^*}(\rho^* u_i^* u_j^*) = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{\text{Re} \text{Re}^*} \left[ \mu^* \left( \frac{\partial u_i^*}{\partial x_j^*} + \frac{\partial u_j^*}{\partial x_i^*} \right) \right] \quad (5-3)
\]

The corresponding energy and species equations are
\[
\frac{\partial T^*}{\partial t^*} + \frac{\partial}{\partial x_j^*}(u_j^* T^*) = \frac{1}{\text{Pr} \text{Pr}^* \text{Re} \text{Re}^*} \left[ \mu^* \left( \frac{\partial T^*}{\partial x_j^*} \right) \right] + \left( \frac{T_a}{T_0} - 1 \right) \frac{\omega}{\rho^* \rho_\infty U} \frac{L}{U} \quad (5-4)
\]

and
\[
\frac{\partial y_i}{\partial t^*} + \frac{\partial}{\partial x_j^*}(u_j^* Y_i) = \frac{1}{\text{Sc} \text{Pr} \text{Sc}^* \text{Re} \text{Re}^*} \frac{\partial}{\partial x_j^*} \left[ \frac{\mu}{\mu_0} \left( \frac{\partial y_i}{\partial x_j^*} \right) \right] - \frac{\omega}{\rho^* \rho_\infty U} \frac{L}{U} \quad (5-5)
\]

Where
\[
\frac{\mu}{\mu_0} = \left( \frac{T}{T_0} \right)^{3/4}
\]

and \( Y_i \) is the species mass fraction and \( \omega \) is the reaction rate. The non-dimensional reaction rate is \( \frac{\omega L}{\rho U} \).

Using the low Mach number approximation, the pressure \( P \) can be written as \( p = p_0(t) + \gamma M a^2 p_1 \) (\( \gamma \) is the ratio of specific heats), \( p_0(t) \) is the total pressure and is constant in the jet simulations. In addition, the equations assumptions are as follows: 1) ideal gas behavior for all species, 2) Newtonian fluid, 3) negligible body forces, 4) zero bulk viscosity, 5) constant and equal specific heat \( C_p \) for all species, 6) Fourier’s law for molecular heat conduction, 7) constant thermal conductivity \( \lambda \), 8) negligible Soret and Dufour effects and
thermal radiation. 9) Fick’s law for mass diffusion and equal mass diffusivities \( D \) for all species. Other assumptions include constant density, unity Lewis number.

### 5.3 Reaction Descriptions

Complex or detailed reaction mechanisms would provide more practical physics, but would increase the code running cost. The one step global reaction setting may not reflect as much complex information as detailed ones; however, our objective is looking for a general conclusion about the flame stabilization mechanism so the one step mechanism is appropriate.

In the jet3d code, a simple global binary reaction is applied

\[
F + O \rightarrow P
\]  

(5-6)

\( F \) represents the fuel, \( O \) represents the oxidizer, and \( P \) represents the product. The reaction rate is given by

\[
\dot{\omega} = A \rho^2 Y_f Y_o \exp\left( \beta \frac{1-\theta}{1-\alpha(1-\theta)} \right)
\]

(5-7)

So the non dimensional reaction rate in the code is

\[
\dot{\omega}^* = \frac{\dot{\omega}}{\rho U} = A \frac{L}{U} \rho Y_f Y_o \exp\left( \beta \frac{1-\theta}{1-\alpha(1-\theta)} \right)
\]

(5-8)
where \( A \) is a constant number with units of \( \frac{m^3}{kg \cdot s} \), \( T_{ad} \) is the adiabatic temperature and \( T_{ac} \) is the activation temperature. The Zel’dovich number, \( \beta \), the heat release factor, \( \alpha \), and the normalized temperature, \( \theta \), are given by

\[
\theta = \frac{T - T_0}{T_{ad} - T_0}, \quad \alpha = \frac{T_{ad} - T_0}{T_{ad}}, \quad \beta = \frac{T_{ac}}{T_0}
\]  

From Equation 5-6, using a linear combinations of fuel and product species, the mixture fraction at any given time and location can be expressed as

\[
Z = Y_F + \frac{Y_F W_F}{W_P} = Y_F + 0.5 \times Y_P
\]  

Then substituting \( Y_P = 1 - Y_F - Y_O \) into Equation 5-10 yields,

\[
Z = 0.5 \times (1 + Y_F - Y_O)
\]  

The stoichiometric value is 0.5. \( Y_F \) is the fuel mass fraction, \( Y_O \) is the oxidizer mass fraction and \( Y_P \) is the product mass fraction. Fuel, oxidizer and product reaction rates are magnitude equal and \( \omega_F = -\omega_F = -\omega_O = \omega \).

### 5.4 Numerical Method of Solving the Governing Equations

The numerical implementation of the low Mach number formulation for the jet simulation is based on the implementation by Boersma’s (1998). The temporal integration of the governing equations is implemented using a predictor-corrector approach. First, the
transport equations are integrated from time level \( n \) with an explicit Adams-Bashforth step to an intermediate level, i.e.

\[
T^* = T^n + \Delta t \left[ 1.5(-A_T + D_T)^n - 0.5(-A_T + D_T)^{n-1} \right]
\]

where \( A_T \) and \( D_T \) stand for the advective and diffusive terms in the energy transport equations, solving \( Y \) is the same method as \( T \). The equation \( P = \rho RT \) is used to get the density for the intermediate condition. Also the momentum equations are integrated into the intermediate condition, i.e.

\[
\rho^* u^* = \rho^n u^n + \Delta t \left[ 1.5(-A_m + D_m)^n - 0.5(-A_m + D_m)^{n-1} \right]
\]

where \( A_m \) and \( D_m \) stand for the advective and diffusive terms in the momentum equations. The intermediate condition of pressure is determined from the pressure Poisson equation, i.e.

\[
\nabla^2 P^* = \frac{1}{\Delta t} \left[ \nabla \cdot (\rho^* u^*) + \frac{\partial \rho^*}{\partial t} \right]
\]

The pressure term is used to derive the corrected \( \rho^* u^* \) as follows:

\[
\rho^* u^* = \rho^* u^* - \Delta t \nabla P^*
\]

Finally, the temperature at step \( n+1 \) is derived using the Adams-Moulton corrector

\[
T^{n+1} = T^n + 0.5 \left[ (-A_T + D_T)^n + 0.5(-A_T + D_T)^* \right]
\]

Then step \( n+1 \) \( \rho^{n+1} u^{n+1} \) is also updated with the Adams-Moulton corrector to
\[ \rho^{n+1}u^{n+1} = \rho^n u^n + 0.5 \left[ (-A_m + D_m)^n + 0.5(-A_m + D_m)^* \right] \]

The species equations of \( Y_i \) are solved using the same methods as those used to solve \( T \), except that the corresponding source terms are different.

The governing equations are spatially discretized on a three-dimensional staggered grid with the aid of a second-order finite volume method for both advective and diffusive terms. No special treatment for the convective terms has been used. The convective term in the transport equation is discretized with a Total Variation Diminishing (TVD) scheme. The computational grid in the \( r \) direction is non-uniform, which allows for an accurate calculation near the orifice without excessive use of grid points in the far field of the jet (Boersma, 1998).

### 5.5 Computational Domain Geometry and Boundary Conditions

The computational domain and boundary conditions are illustrated in Figure 5.2. The jet fluid (in general fuel) is injected along a slower co-flowing air (oxidizer) stream. The co-flow velocity is typically very low compared to the jet velocity.

As suggested by Han and Mungal (2000), the velocity of the stoichiometric contour can be estimated and used to approximate the amount of mixing between the fuel jet and the surrounding air. This velocity, \( u_s \), can be calculated from

\[ u_s = z_s U_0 + (1-z_s)U_{cf} \]  

(5-12)
where $z_s$ is the stoichiometric mixture fraction, $U_0$ is the nozzle exit velocity, and $U_{cf}$ is the co-flow velocity. The flame models two aspects of velocity behavior: First, if the flame base velocity is larger than $u_s$ then the flame blows out. Second, blow-out is sensitive to the co-flow speed. Since the stoichiometric mixture fraction for most hydrocarbon fuels is small, the stoichiometric velocity is highly weighted by the co-flow speed. However, the simulations in this chapter only involve a global one step reaction. $z_s$ is 0.5 and so co-flow weighs the same as jet inlet velocity within the flame.

![Figure 5.2 Schematic of computational domain with boundary conditions.](image-url)
There are three types of boundaries in the code: the inflow, outflow, and lateral boundary. At the inflow, $u_r = U_0 \cos \theta$, $u_\theta = -U_0 \sin \theta$ in the orifice and elsewhere $u_r = U_{\text{coflow}}, u_\theta = 0$. In addition, $u_\phi = 0$ everywhere, the outflow and lateral boundary are traction free and convective boundary (Boersma 1998), respectively.

5.6 Simulation Results

The simulations are based on the inlet conditions of Re=2500 based on the fuel inlet conditions and jet diameter with $U_0 = 10$. Co-flow is set as 0.2 and the turbulent intensity is given by 5%. The fuel and oxidizer concentrations are specified by $Y_F = 1, Y_o = 0$ in the orifice while $Y_F = 0, Y_o = 1$ at the co-flow. In the initial flame zone (pilot extension domain), they are set as $Y_F = Y_o = 0.01$. The constant value of $A \frac{L}{U}$ is set as $4 \times 10^5$. The heat release parameter $\alpha$ is 0.8 and the Zel’dovich number $\beta=3.0$. The mesh resolution is $600 \times 120 \times 12$ and Re number is 2500. The computation was carried out on 6 processors HPC facility at NC State University. The maximal time step is set to $10^{-4}$, but is automatically decremented at every step. The resolution of direction $z$ satisfies the minimum requirement for code running and its effect on the 2D output is ignored. All results are output in the $x$-$y$ plane.

The calculations were run sufficiently long to be independent of the initial conditions. Figure 5.3 shows the 2D output results. Figure 5.3(a) is the temperature distributions. Clearly, the flame shows symmetric shape before the flames merge together from the left and right.
sides downstream. Figure 5.3(b) is the normalized flame index (N.F.I) which is calculated using the same methods as used in Chapters 4:

$$N.F.I = \left[ \frac{(z-z_s)}{|z-z_s|} \cdot \frac{1}{2} \left( 1 + \frac{\nabla Y_F \cdot \nabla Y_O}{|\nabla Y_F \cdot \nabla Y_O|} \right) \right] + 2 \quad (5-13)$$

The mixture fraction is defined by Equation 5-11. The flame base structure shows the lean premixed (with N.F.I. value of 1), the rich premixed (with N.F.I. value of 3) and the diffusion flame branches (with N.F.I. value of 2). The solid line represents the stoichiometric mixture fraction with a corresponding value of 0.5 passing through the flame edge along diffusion flames. Flames downstream in Figure 5.3(b) still remain the premixed lean and rich flames. Figure 5.3(c) is the reaction rate near the flame base. The edge shape is characteristic of a fundamental triple flame structure, and indicates that the flame base is partially-premixed. The largest values of the reaction rates are located at the flame edges and they decrease downstream as the combustion mode transitions to a non-premixed flame mode. The findings are consistent with the observation in Chapter 2. Also, this is consistent with the findings that flame bases have the highest heat release rates and are responsible for stabilizing the entire flame. The conclusion is the same as the shear layer flame DNS simulations in Chapter 4. Namely, the flame is stabilized by the partially-premixed flame stabilization mechanism.

Figure 5.3(d) and (e) clearly show that the left and right leading edges are located at the non-dimensional height of 7.78. The initial inlet position starting as 7.616 and then the lift-off height is around non-dimensional 0.26, which occupies 32 grids. Because of the
transition flow, the flame edge position fluctuation is not seen and lift-off heights are constant.

The transition physics makes the flow symmetric. This can be seen in the portion of Figures 5.3(a) before the downstream flame interaction and in Figure 5.3(b) where the vortex shapes are consistently paired and symmetric eddies. But in contrast with their downstream neighbors, the flame bases exhibit no vortex structures. This indicates that the flow near flame edges is laminar rather than turbulent. This profile is quite similar to Figure 5.1, but the extent of the laminar flow part is significantly reduced and the flame base widens slightly. This may be explained by the lift-off behaviors.

Figure 5.3(a) and (b) shows eddies in the flame zone, but the eddy magnitudes are not clear. While Figure 5.4 represents large eddies with vorticity distributions in the xy plane. Dark blue and red color zones represent the minimum and maximum vorticity magnitudes, respectively, where the non-dimensional values are as large as 800 in Figure 5.4 (a). Figure 5.4 (b) shows the relative positions of the flame edges with respect to the vorticity field. The vorticity magnitudes at the flame edges are less than 50, which indicate that there are no large eddies on the flame edges. Moreover, the results are a stable condition and the relationship will not change. Therefore, the large eddy theory cannot be explained as the stability mechanism for lifted jet flames.
Figure 5.3 (a) Temperature distributions, (b) Normalized flame index, (c) Reaction rate structure at the flame base, (d) The left flame edge position and (e) The right flame edge position.
Figure 5.4 (a) Vorticity distributions in the $xy$ plane and (b) Flame edge relative positions on the vorticity fields.
5.7 Conclusions

In this chapter, a lifted jet flame simulation using a DNS method under a transitional flow with a Re number of 2500 was performed. Although, the full range of turbulent scales are not explored within the computations since the flow is transitional, the results serve to illustrate the role of large-scale eddies on flame stabilization. The types of large-scale instabilities in the transitional flow regime are expected to persist even at higher Reynolds numbers.

The 3D results exhibit more-or-less symmetric profiles associated with the predominance of 2D instabilities. Therefore, only profiles along the axi-symmetric planes are presented. The results show a similar transition profile to Takeno’s results (Takeno 1994). With the prescribed mixture strength, lifted flame conditions are obtained. The flame achieve a stable lift-off position and exhibit a partially premixed, triple flame structure. It is found that the large eddies does not play a significant role in the flame stabilization, a trend that is counter to the large-eddy model discussed in Chapter 1. On the other hand, this simulation proves that a stabilizing lifted jet flame under a transitional flow is also controlled by the partially premixed stability theory which is developed by the study of triple flames.
Chapter 6. RANS Investigation of Lifted Jet Flames’ Stabilization

In this chapter, the mean structure, stability and the lift-off heights of lifted methane-air flames in a turbulent round jet are computed using the Reynolds-averaged Navier-Stokes (RANS) approach coupled with the Eddy-Dissipation Model (EDM) model for combustion. The computations are based on a 5-step methane-air reduced mechanism. The simulation results show that the EDM model does reproduce a mean partially-premixed flame structure at the leading edge of the lifted flame and predicts the lift-off heights reasonably well compared to published experimental results. Implications of the use of the EDM concept for partially premixed flames are presented.

6.1 Introduction

Lifted flames are very common in many fire scenarios, such as in pool fires (Joulain 1998, Miller et al., 1998, Takahashi et al., 2001) and the modeling of jet flames is still a major project in studying lifted jet flame (Cleaver et al., 2003, Cumber et al., 2006, Onokpe et al., 2009). Lifted jet flame is a common phenomenon resulting from a pipe leaking. This kind of flame stability mechanism involves a partially premixing of fuel and oxidizer. Also, incipient fire is typically developed by the partial premixing of fuel and oxidizer. The two kinds of fire safeties are related to lifted jet flame and it is necessary to investigate the lifted
jet flame stability. Furthermore, the modeling of lifted jet flames includes the physics of the entire flame propagating and aids us to understand how flame spreads spatially.

The stabilization mechanisms of turbulent jet lifted flames have been widely studied. Various theories advanced different mechanisms for lifted flame stabilization (Pitts 1988, Lyons 2007, Lawn 2009). Numerical simulations also offer different interpretations of the stabilization mechanisms. In their 2-D DNS results, Kaplan et al. (1994) and Montgomery et al. (1998) argued that the flame base moves up with the vortex to which it is attached, and then quickly jumps upstream to attach to a new lower one periodically. Luo (2003) also used 2-D DNS to model a fuel jet surrounded by a hot co-flowing stream and reported triple flame-like structures at the lifted flame base, while large-scale vortex structures have relatively small effects on the lifted flame stability.

Large Eddy Simulations (LES) of lifted flames have also offered different interpretations of the stabilization mechanisms. Jones and Navarro-Martinez simulated an H₂/air jet case (Jones et al., 2007), and with a co-flow of 1035–1045 K, concluded that auto-ignition and the formation of HO₂ are the main mechanisms of stabilization. Domingo et al. (2008) simulated a CH₄/air jet case with a 1350 K co-flow and again identified auto-ignition, in this case originating in the lean region of the jet. Another LES study, by Ferraris and Wen (2007) used the partially premixed combustion model by Domingo et al. (2002) with a freely propagating one-dimensional premixed flame submodel for the premixed regime and the strained counterflow diffusion flame configuration for the nonpremixed part. They captured the double flame structure, showing a configuration similar to that of the experiment, which
involves a rich premixed branch at the jet center and a diffusion branch at the outer region, both converging the so-called triple point at the flame base. Very few simulations based on RANS are reported in the literature. In a recent study, Kumar et.al (2007) observed that flame stabilization occurs at a point near the stoichiometric mixture fraction surface, where the local flow velocity is equal to the local flame propagation speed.

While various models for flame stabilization have been available for some time in the literature, there is little consensus on the choice of the appropriate combustion models that can reasonably predict the structure and dynamics of the leading edges of the lifted flames; these edges hold the key to flame stabilization. The choice of the particular combustion model can be critical, since the modeling of large-scale fires can result in computationally demanding simulations. Many industrial applications using commercial computational fluid dynamics (CFD) codes rely on variants of the eddy-dissipation model (EDM), which was originally developed by Magnussen and Hjertager (1976). The EDM approach is based on the principal assumption that chemistry is much faster than the rate of turbulent mixing; and therefore, the rate of reaction and heat release are strongly dependent on the limiting process of turbulent mixing. It has long been argued that the inherent assumptions of the EDM make it suitable only for a limited subset of combustion problems, such as in non-premixed flames (1989).

The potential challenge of addressing the leading edge of a lifted non-premixed flame may be the result of its partially-premixed nature. In fact, an increasingly popular theory of lifted flame stabilization argues that that the partially-premixed nature of the leading edge
allows for both the ability of this edge to propagation upstream and its attachment to the diffusion flame that trails. Within the context of partially-premixed flames and the EDM, a recent study by Cabra et al. (2002) show that the EDC model, a more recent variant of EDM, predicts the lift-off of the turbulent non-premixed H₂/N₂ jet flame in a vitiated flow. While the lift-off heights based on the EDC were slightly under-predicted, results show that the overall structure of the leading edge based on OH are similar qualitatively to those of the experiment.

The objectives of this investigation are to use the EDM combustion model with the RANS approach to compute the basic structure, albeit in averaged form, of lifted flames with co-flow air and examine the agreement of lift-off heights with experimental data. Moreover, we use scalars and velocities at leading edges of the lifted flame edges to investigate their structures. The velocities found are compared to the laminar averaged premixed flame speeds and the variation of the velocities through the reaction edge zone is investigated.

6.2 Problem Configuration and Numerical Implementation in CFX

6.2.1 Geometry and mesh construction

The computations are based on a lifted jet diffusion flame in co-flow air with an inlet diameter for the fuel jet of 4 mm. The computational configuration is shown in Figure 4.1. The domains are 100 mm x 300 mm in the axial x and y directions with a symmetry boundary and 5 degree rotation about the y-axis. The co-flow wall is 100 mm deep from the
jet nozzle. A dense grid is assigned in and around the flame zones to resolve the mean flame structure. The number of computational is 48,229 with a mesh minimal resolution angular of 30 degree. The minimum edge length is 0.4 mm and the maximum edge length 4mm in non-flame zones. The length scale is uniform 0.6 mm in flame zone while it is refined to uniform 0.3 mm in flame edge zone.
Figure 6.1 Geometries and meshes of the computational domain. Flame zone’s mesh edge length is uniform 0.6 mm and flame edge domain’s mesh edge length is uniform 0.3 mm.
6.2.2 Boundary and initial configuration

Uniform velocity conditions are applied for both fuel and co-flow boundaries. A velocity boundary condition is zero for free jet cases or 0.18 m/s for co-flow jet cases, which are applied for the air inlet at ambient conditions. A static pressure for entrainment is defined at the inlet boundaries. The fluid is air at 300 K and 101,325 Pa. A free slip and adiabatic wall boundary condition is imposed at the co-flow wall and jet pipe. A uniform temperature of 800 K is set in the whole domain initially in order to initiate combustion and the flame, and then changed back to 300 K at subsequent iterations of the solution once flames are ignited.

6.2.3 Combustion and flow models

The simulations are executed using the commercial computational fluid dynamics (CFD) code CFX 11.0 (CFX, 2004). The combustion closure is implemented using the EDM model, while the turbulence is implemented using the standard k-ε model. The standard k-ε governing equations are

\[
\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho U k) = \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right) + P_k - \rho \varepsilon \quad (6-1)
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \nabla \cdot (\rho U \varepsilon) = \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_{\varepsilon}} \right) \nabla \varepsilon \right) + \frac{\varepsilon}{k} (C_{\text{eq}} P_k - \rho \varepsilon C_{\varepsilon 2}) \quad (6-2)
\]

\[
P_k = \mu_t \nabla U \cdot (\nabla U + \nabla U^T) - \frac{2}{3} \nabla \cdot U (3 \mu_t \nabla \cdot U + \rho k) \quad (6-3)
\]

\[
\mu_t = C_{\mu} \rho \frac{k^2}{\varepsilon} \quad (6-4)
\]
where, the closure constants of $C_\mu, C_{\varepsilon_1}, C_{\varepsilon_2}, \sigma_k, \text{and} \ \sigma_\varepsilon$ are listed below:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_\mu$</td>
<td>0.09</td>
</tr>
<tr>
<td>$C_{\varepsilon_1}$</td>
<td>1.44</td>
</tr>
<tr>
<td>$C_{\varepsilon_2}$</td>
<td>1.92</td>
</tr>
<tr>
<td>$\sigma_k$</td>
<td>1.0</td>
</tr>
<tr>
<td>$\sigma_\varepsilon$</td>
<td>1.3</td>
</tr>
</tbody>
</table>

The equation of transport for component $i$, with a Favre-averaged mass fraction $\tilde{Y}_i$ is:

$$
\frac{\partial (\rho \tilde{Y}_i)}{\partial t} + \frac{\partial (\rho \bar{u}_j \tilde{Y}_i)}{\partial x_j} + \frac{\partial (\rho u_j' Y_i' \tilde{Y}_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_i \frac{\partial \tilde{Y}_i}{\partial x_j} \right) + \bar{S}_i
$$

(6-5)

Where the source term $\bar{S}_i$ is due to the chemical reaction rate involving component $i$. The operators, “$\overline{\phantom{\nu}}$” and “$\tilde{\phantom{\nu}}$”, denote Reynolds averaging and Favre averaging, respectively. The rate of production $\bar{S}_i$ (CFX 2004), for component $i$ can be computed as the sum of the rate of progress for all participating elementary reactions:

$$
\bar{S}_i = W_i \sum_{k=1}^{K} (v''_{ki} - v'_{ki}) R_k
$$

(6-6)

where $v''_{ki}$ and $v'_{ki}$ are the stoichiometric coefficients for component $i$ in the elementary reaction $k$. $W_i$ is the molecular weight and $R_k$ is the elementary reaction rate of progress for reaction $k$, which in ANSYS CFX can be calculated using the EDM and expressed as a minimum of two expressions for $R_k$:

$$
R_k = A \frac{\varepsilon}{k_T} \min \left( \frac{[i]}{v_{ki}} \right) \quad \text{and} \quad R_k = AB \frac{\varepsilon}{k_T} \min \left( \sum_p \frac{[i]W_i}{v'_{ki} W_i} \right)
$$

(6-7)
where \([i]\) is the molar concentration of component, \(i\), which only includes the reactant component for the first expression; while, the second expression involves sums over products, as indicated by the parameter \(P\). The number \(A\) may be a constant number or modeled as a variable. In our simulations, only \(A\) is active. The simulations use the second order backward Euler transition and time dependent scheme. All solving results are incompressible solutions. The required convergence condition is the r.m.s of \(1\times10^{-4}\).

The fluid time scale is defined by \(\tau_f = k_T/\varepsilon\). Here, \(k_T\) is turbulent kinetic energy and \(\varepsilon\) is the dissipation rate of turbulent kinetic energy. In these simulations, chemical time scale reference \(\tau_c\) is set as 0.0005 s (CFX 2004). Local extinction occurs when \(\tau_f < \tau_c\) and temperature below 600 K (Horvat et al., 2007). Mixing rate limit is 300 s\(^{-1}\). Turbulence closure is achieved using the model of standard \(k-\varepsilon\) and turbulence intensity is 5\%. The inlet boundary of \(k\) and \(\varepsilon\) is calculated using

\[
I = \frac{u'}{u} = 5\%, k_{inlet} = \frac{3}{2} \bar{u}'^2 \quad \text{and} \quad \varepsilon_{inlet} = \rho C_{\mu} \frac{k^2}{\mu_t} \tag{6-8}
\]

Otherwise, at the opening boundaries, the conditions are set as turbulent gradients as zero. The reaction mechanism is based on 5- step reduced mechanisms (CFX 2004) for methane oxidation:

\[
\begin{align*}
\text{Reactions 1 and 2} & \quad \text{CO}_2 + \text{H}_2 & \xrightleftharpoons[\text{R}_2]{\text{R}_1} & \text{CO} + \text{H}_2\text{O} \\
\text{Reaction 3} & \quad 2 \text{CO} + \text{O}_2 & \xrightarrow{\text{R}_3} & 2 \text{CO}_2 \\
\text{Reaction 4} & \quad 2 \text{CH}_4 + \text{O}_2 & \xrightarrow{\text{R}_4} & 2 \text{CO} + 4\text{H}_2 \\
\text{Reaction 5} & \quad 2 \text{H}_2 + \text{O}_2 & \xrightarrow{\text{R}_5} & 2 \text{H}_2\text{O}
\end{align*}
\]
6.3 Results and Discussions

First series simulations are jet flames with a co-flow of 0.18 m/s. Five cases under the series with jet exit velocities of 19.66 m/s (case A), 23.09 m/s (case B), 25.4 m/s (case C), 31.27 m/s (case D) and 38.4 m/s (case E), respectively, achieve stable lifted jet flames. The corresponding experimental flame height data by Terry and Lyons (2005) are 0.635 cm, 0.95 cm, 1.27 cm, 2.86 cm, and 3.81 cm, which are measured based on chemiluminescence. In the simulations, the coefficient \( A \) in Equation 6.7 is set to different values in each case so that the lift off height differences compared to experimental data remain very small. Thus, \( A \) is modeled by connecting the different values. The simulation lift-off heights are 0.645 cm, 0.974 cm, 1.25 cm, 2.84 cm and 3.77 cm, respectively. These heights are measured, according to Figure 6.2 method, from the jet nozzle to the lowest position of 1% maximum bound of methane oxidization reaction rate \( R_4 \) contour.

The second series are the free jet flame simulations, four cases with jet exit velocities of 25.4 m/s (case A1), 31.27 m/s (case B1), 38.4 m/s (case C1) and 44.37 m/s (case D1) are implemented. The lift off heights measurement method is the same as the first co-flow series simulation cases. The coefficient \( A \) values are calculated using the previously modeled \( A \) profile.
Figure 6.3 illustrates the flow dynamics around the lifted flame leading edge. Solid curved lines are streamlines around this edge. Also shown are contours of the temperature to indicate the flame position. The right-hand side of the figure corresponds to the fuel jet side, and the left-hand side corresponds to the co-flow air side. The figure shows air entrainment to the fuel side prior even to reaching the flame edge; therefore, the mixture ahead of the leading edge of the lifted flame is partially premixed. The dotted line in Figure 6.3 delineates the streamlines turning points, which indicate important flow altering events near the lifted flame leading edge. The lines indicate two important events within this region, one associated with the co-flow air entrainment upstream of the leading edge, and the second associated with the presence of the flame. The streamlines also indicate the presence of flow.
divergence ahead of the flame edge and its convergence behind the flame edge consistently with previous observations of laminar triple flame structures (Ruetsch et al., 1995).

Figure 6.4(a) is a co-flow case streamlines while Figure 6.4(b) is a free jet case; both cases have the same jet inlet velocity of 25.4 m/s. From the streamline curvatures, the streamlines in the free jet case show clearly steeper curvatures than corresponding ones in the co-flow condition. This may be explained that inertia force in co-flow conditions decreases the streamline curvatures.

![Figure 6.3](image)

**Figure 6.3** Flow divergences around the lifted flame leading edges. Solid lines represent streamlines and bold dashed lines represent flow divergence.
Figure 6.4 (a) Streamlines distribution in case C with a co-flow of 0.18 m/s and (b) Streamlines of a free jet flame case A1.
Using the case E as an example, Figure 6.5 shows the typical contour of velocity magnitudes and indicates an acceleration of the flow, especially on the fuel-lean side, as observed in typical triple flame structures (Ruestsch et al., 1995). All other cases have the same trend of profile in the simulations. Therefore, the flow patterns are consistent with laminar flame edge profiles reported in the literature, suggesting a degree of partial premixing ahead of the flame edge and flow divergence and acceleration across this edge. Although, identifying a fine-scale triple flame structure in a turbulent flame edge is far from being resolved in a RANS computation, a similar, but mean, structure is being constructed with the present computational approach. We ascertain that the presence of this structure is
what establishes the stabilization mechanism for the turbulent lifted flame in our computations.

Figure 6.6 Flame edge structures: Normalized Flame Index (N.F.I) on reaction rates $R_4$. (a) to (e) are the jet flame cases with a co-flow of 0.18 m/s, while (f) to (i) are free jet flame cases.
In lifted flames, the extent of the premixed region ahead of the flame edge can be relatively small depending on the liftoff height. Consequently, it can be difficult to distinguish the reaction zones visually. Here, we attempt to distinguish the different branches of non-premixed and premixed lean and rich burning in the flame by using the flame index (Andrew et al., 2005), which is defined as:

\[
FI = \frac{Z - Z_S}{|Z - Z_S|} \left[ 1 + \frac{\nabla Y_F \cdot \nabla Y_O}{\nabla Y_F \cdot \nabla Y_O} \right]^{\frac{1}{2}}
\]

(6-9)

Here, \(Y_F\) denotes the fuel mass fraction and \(Y_O\) the oxidizer mass fraction. \(Z\) is the mixture fraction, and \(Z_S\) is the corresponding stoichiometric value. For the present fuel-air mixture, the stoichiometric mixture fraction is 0.055. Therefore, the rich and lean premixed zones are located in the inner and outer regions in which the local mixture fraction \(Z\) is larger and smaller than \(Z_S\), respectively. The mixture fraction is defined following Bilger expression (Bilger et al., 1990).

\[
Z = \frac{2(Y_c - Y_{c,o})}{W_c} + \frac{Y_h - Y_{h,o}}{2W_h} - \frac{Y_o - Y_{o,o}}{W_o}
\]

\[
\frac{2(Y_{c,f} - Y_{c,o})}{W_c} + \frac{Y_{h,f} - Y_{h,o}}{2W_h} - \frac{Y_{o,f} - Y_{o,o}}{W_o}
\]

(6-10)

where \(W_i\) is the molecular weight of the \(i\)th element (carbon, c, hydrogen, h and oxygen, o). Subscripts (f) and (o) refer to the fuel and air streams, respectively. With this definition \(FI = 1\) for the rich premixed zone, \(-1\) for the lean premixed zone, and \(0\) for nonpremixed zone.

In order to distinguish flame and non-flame zones, a normalized flame index, N.F.I., is used,
where \( NFI = FI + 2 \). Accordingly, a value of unity for \( NFI \) corresponds to lean premixed branch, 2 for diffusion zone and 3 for rich premixed branch. Moreover, a zero value is reserved for a non-combustion zone. Figure 6.6 shows the N.F.I for all series simulations flame structures. The contours for N.F.I are based on a threshold of 1\% or more of the methane consumption reaction, \( R_4 \). All contours corresponding to the different exit velocities show the presence of lean premixed and rich premixed flame branches, respectively, on the air and fuel sides, respectively. As the lifted off height and, accordingly, the exit velocity increases, the extent of the lean branch increases in the first series simulations (from case A to case E) of a co-flow 0.18 m/s cases. However, in the other series of free jet cases, the lean branches do not have significant changes as jet inlet speed increases.

Having established the presence of a triple point in the mean structure of the leading edge, we revisit the velocity information discussed earlier. Figure 6.7 tracks the velocity variations along flame edges as a function of the position along the streamlines passing through the triple point. Figure 6.7 (a) is for co-flow jet flame cases while Figure 6.7(b) shows the free jet flame cases. The flame edge in the inlay of Figure 6.7 is indicated by reaction rate \( R_4 \) contours. As indicated by the divergence and the convergence of the streamlines shown in Fig. 6.3, 6.4 and 6.5, the velocity magnitudes firstly decrease then increase. The increase may be attributed primarily to the flow acceleration behind the flame edge; although, some flow convergence is present as well. The velocity ratios of the flame edge velocity and flame propagation speed are averaged at 2.58 for co-flow jet flames and 2.43 for free jet flames. That is very close to the methane air laminar triple flame structure. In
addition, the flame edge velocity always larger than laminar flame speed which is consistent with our experimental findings in Chapter 3. The velocity variation profiles move up as the Re number increases for both co-flow and free jet flame simulations.

Figure 6.8 compares the lift-off heights based on the computed and measured values as functions of the exit jet velocities. Co-flow lifted jet flame simulations are used to model the coefficient A in the EDM model. Keeping the lift off height errors between the co-flow jet flame simulations (symbols “o”) and experiments (symbols “+”) less than 2.5% (Figure 6.8 (a)), we find that A is a parabolic profile with the jet exit velocity, which is shown in Figure 6.8(b) using a solid line connected by symbols “□”. The values are 6.9, 6.2, 5.7, 4.6 and 4.6 respectively in the 5 co-flow jet flame cases. Values of symbols “Δ” on the profile are 5.58, 4.86, 4.52 and 5.02, which are chosen for the four free jet flame case simulations.

For free jet lifted flame simulations, each case also achieves stable lifted jet flames, and the lift-off heights are 1.24 cm, 1.63 cm, 2.02 cm and 3.35 cm, respectively. These heights are measured from the jet nozzle to the lowest position of 1% maximum bound of methane oxidization reaction rate R4 contour. The corresponding experimental flame height data by Terry and Lyons (2005) are 1.27 cm, 1.52 cm, 1.91 cm and 3.18 cm, which are measured based on chemiluminescence.

Figure 6.8(c) shows a good agreement between the computed and experimental measured values. The correlations coefficients squares for the experimental and computed lift-off heights, R², are 0.8659 and 0.8875, respectively. The experimental lift-off heights and the computed lift-off heights yield slopes of 0.093 and 0.1021, respectively, and intercepts of
-1.2443 and -1.4675 cm, respectively. Both trends are consistent with the scaling argument presented by Peters (2000).

To summarize the trends observed so far based on the leading edge structure and dynamics, the various observations are consistent with the flame edge structure reported in the literature for laminar flames:

- Ahead of the flame edge, flow streamlines diverge and then subsequently converge downstream of this edge.
- The divergence and convergence of the streamlines are accompanied by a short deceleration, followed by acceleration. The acceleration is attributed primarily to heat release in the flame.
- The flame structure, albeit in averaged form, exhibits lean and rich premixed and diffusion branches that are characteristic of triple flames and edge flames. The presence of the different branches resourced from triple flame structure serves as a stabilization mechanism for the lifted jet diffusion flames.

At this point, it is interesting to provide an interpretation of how the EDM model is able to provide a stabilization mechanism for the lifted flame and how this model may contribute to very good predictions of the flame lift-off height. Here we ascertain that an important part of the answer lies in the governing equations, which by adopting an eddy viscosity model look essentially similar to the (non-averaged) instantaneous equations for continuity, momentum, species and energy. The EDM model serves primarily to broaden the
reaction zones, without altering what the averaged governing equations are doing. This broadening is consistent with the averaging done on the transported variables as well. Therefore, the EDM model in the context of a RANS formulation emulates the trends of a laminar fine-scale formulation based on instantaneous equations resulting in a partially-premixed edge flame.

The linear correlation obtained for the lift-off height with the jet exit velocity in computed data, and consistently observed in experimental data, may be attributed to a scaling argument that has been advanced recently by Peters (2000). This scaling is consistent with the EDM principle of rate-limiting role of turbulent mixing on chemistry (the so-called high-Damköhler number limit of fast chemistry). The analysis yields an expression of the form:

\[ H \sim u_0 Z_s \frac{D}{S_L^2} \]  

(6-11)

where \( H \) is the lift-off height; \( u_0 \) is the exit velocity; \( D \) is a diffusivity coefficient, such as the kinematic viscosity; and, \( S_L \) is the laminar flame speed at stoichiometric conditions.
Figure 6.7 (a) Velocity magnitude variations along the flame edges of case A to case E. (b) Velocity magnitude variations along the flame edges of case A1 to case D1.
Coordinate Y (m) of case A

Velocity=19.66m/s
case A

Velocity=23.09m/s
case B

Velocity=25.4m/s
case C

Velocity=31.27m/s
case D

Velocity=38.4m/s
case E
<table>
<thead>
<tr>
<th>Coordinate Y (m) of case A1</th>
<th>Velocity (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1128</td>
<td>0.1134</td>
</tr>
<tr>
<td>0.1134</td>
<td>0.114</td>
</tr>
<tr>
<td>0.114</td>
<td>0.1146</td>
</tr>
<tr>
<td>0.1146</td>
<td>0.1152</td>
</tr>
<tr>
<td>0.1152</td>
<td>0.1158</td>
</tr>
<tr>
<td>0.1158</td>
<td>0.1164</td>
</tr>
</tbody>
</table>

Jet Velocity:
- Case A1: 25.4 m/s
- Case B1: 30.08 m/s
- Case C1: 38.4 m/s
- Case D1: 44.37 m/s
Figure 6.8 (a) Lift off height comparisons for co-flow jet flames. (b) Modeling the coefficient A in the EDM model. (c) Lift off heights comparisons for free jet flame cases.
A values

Velocity (m/s)

Coflow jet flame cases
Free jet flame cases

\[ y = 0.0087x^2 - 0.6369x + 16.148 \]
6.4 Conclusions

The structure and dynamics of lifted non-premixed methane-air flames at different exit velocities are studied numerically using a RANS formulation, including the EDM model for combustion closure and the standard k-ε model for turbulence closure. The results show that the model achieves a lifted flame structure as observed in experiments. The lift-off mechanism is attributed to the nature of the governing equations, which tend to emulate the
instantaneous equations at the same conditions with a broadening of the reaction zone by the EDM approach.

The results also show that the computed lift-off heights are in very good agreement in both trends and magnitudes with experimental measurements. The observed linear trends are consistent with physical arguments that are valid for fast chemistry and, therefore, applicable to the experimental conditions and consistent with the EDM model. The mean flame edge structures all exhibit triple flame structures of premixed lean, premixed rich and diffusion branches, which is consistent with our DNS simulation results.

Therefore, the results show that despite the model simplicity, the EDM approach may provide reasonable predictions at conditions of partially-premixed combustion. While, fast chemistry has been a common assumption in the prediction of fires, it was not clear if the EDM would provide a strategy for predicting lift-off heights of flames as well. However, modeling the coefficient of $A$ in Equation 6-7 may be considered as a good method to develop the EDM model and such that predict lift off height.

A more important argument to advance is whether there is a need for a more sophisticated predictive strategy for turbulent combustion where the overall prediction depends also on how well the other models (e.g. turbulence, radiation) are executed and how much uncertainty is associated with the initial and boundary conditions of the problem.
Chapter 7. Conclusions and Recommendations for Future Work

7.1 Conclusions

In this study, flow characteristics and flame structures are used to investigate the stabilization conditions of turbulent lifted jet flames. Both experimental methods and simulations are applied. In experiments, an optical CH filtered and intensified high speed camera system is used to visualize the methane air lifted jet flame base structures. All lifted stable, reattachment and blowout flame phenomena are discussed; A PIV method with Nd:YAG lasers is used to investigate the flame edge zone and flow fields. Meanwhile, one DNS method based on the S3D (from Sandia National Laboratory) is applied to study the hydrogen air lifted shear layer flames. Another DNS method of Jet3d is used to simulate a low Re number jet flame. Finally, the RANS method with the EDM model using ANSYS-CFX is employed to simulate lifted methane air jet flame with many different Re number conditions. All results support that flame edges are in partially-premixed conditions and exhibit triple or edge flame structures. Also, the velocity variations through flame edges as well as streamline divergences are congruent with the features of triple flames. The edge flame theory is fully supported by this research and is substantiated by both experimental and computational data. It can best explain the turbulent lifted jet flame stability.
In addition, this research finds no necessary relationship between large eddies and lifted jet flame edges. We conclude that the large eddy theory cannot explain the flame stabilization. Also, our research results do not find evidence to support other potential flame stability theories such as fully premixed theory, turbulent intensity theory, and auto-ignition theory.

7.1.1 Experimental Findings

The methane-air lifted turbulent jet flame bases are visualized using CH chemiluminescence. It is found that the reaction zones at flame bases are thick and intense compared to downstream. Flame bases are shaped like stretched triple flames; therefore, they are in partially premixed conditions. The stable lifted jet flames under three different Re numbers always have stable \( \text{CH}^* \) grayscale quantities, which imply that lifted stable flame bases require a constant energy where the reaction rates are maximal. The particular steep heat release gradients between flame edges and downstream flames are also consistent with triple flames structures observed in the literature.

Flame holes are found to play a role in perturbing the flame base structure and the flame base stability. As the flow rate increases, flames holes are more prevalent and are generated closer to the flame base. Under very high flow rates the flame holes are expected to entirely occupy the flame base and potentially contribute to flame blow-out.

During the transitional process of flame reattachment, the flame base holds stable higher energy regions locally and stabilize the flame until the flame attach to the jet nozzle rim. Once the flame attaches to the jet nozzle, the heat release distribution is a pure laminar
diffusion pattern. Meanwhile, the flame blowout process proves that flame bases are unstable. Although heat releases still show large values at the flame edge compared to downstream flame, they are unstable and decrease gradually, finally result in the entire flame extinguish.

In addition, the flow characteristics are studied using a PIV method with Nd:YAG lasers. A new method based on chemiluminescence grayscales second derivatives was used to achieve accurate flame zones successfully. The velocities at methane air lifted jet flame edges under a Re number of 4790 are probed. It is found that two velocities are important: one is the flame edge velocity, which is larger than the corresponding laminar flame speed; the other is the flame propagation speed. The two velocity magnitude variations through flame edges are consistent to the triple or edge flame characteristics. Also, streamline divergences of lifted flame bases are the same as triple flames. The vorticity distributions as well as the streamline profiles at flame edges show that the large eddies have no necessary relationships with flame edges. Thus we conclude that the large eddy stabilization theory cannot explain the lifted jet flame stabilization.

7.1.2 Simulation Conclusions

All simulation results including flow characteristics and flame base structures agree well with the experimental findings.

The unsteady shear layer hydrogen air flame in a DNS method shows a triple flame structure. The displacement speed, along with the streamline characteristics, illustrate that the flame base is moving together and plays a role to stabilize the flame. The merging of
premixed lean and diffusion flame downstream does not change the heat release distributions, which is also consistent to our experimental findings.

In addition, the lifted jet flame with a low Re in a DNS proves that the flame edge is still a triple flame under the transitional condition. The flame base is located rather in a laminar flow part where large eddies have no influence; therefore, the triple flame structure is responsible for the flame’s stability.

Finally, the CFX-RANS simulations of methane air lifted jet flames demonstrate that the mean structures of lifted jet flame bases are triple flames. This method also proves that the EDM model can efficiently model turbulent diffusion jet flames. Velocity magnitudes decrease then increase to pass through the flame edges, which is consistent with a triple flame. The velocity variation ratios agree well with our experimental results and also agree well with triple or edge flame characteristics. Therefore, the stability mechanism is governed by the triple flame stability mechanism.

7.2 Recommendation for Future Work

There are some related studies, both in experimental and numerical aspects, which are of great interest in understanding lifted flames. Some of these studies have not been performed due to the difficulty of the experiment or extremely high computational cost. However, recent advances in experimental techniques and computational speed make these studies more achievable.
7.2.1 Experimental investigation of 3D lifted jet flames

Turbulent lifted jet flames are a 3D phenomenon. Under high Re conditions, each direction has significant effects on flame structures. Planar 2D or projected 2D images lose information; whereas, 3D experimental data is the most complete. 3D experiments can be implemented by planar measurements with the gradient normal to the plane (Su and Clemens 1999; Kähler and Kompenhans 1999) or with crossed multiple planar LIF measurements (Karpetis et al., 2003; Fujisawa et al., 2007; Ueda et al., 2009).

Also, higher resolution images are needed to investigate the flame base at high Re values since the flame base shape is more complex. Alternative reaction zone markers such as CH₂O-OH and CO-OH are proposed. Especially, CH₂O-OH tends to align well with the heat release region, and also represents a main path of hydrocarbon oxidation. Further, simultaneous PIV and CH₂O-OH PLIF in a flame would be possible with current advances in imaging techniques.

7.2.2 Experimental investigation of flame base structures by varying fuel composition

Using diluted fuel, the lifted jet flame base structures would vary with the fuel mass fractions. The experiments would find how the flame structures change with different dilution types and ratios, as well as how the velocity field varies at the flame edges. This would provide a more complete study of flame edge behavior and characteristics. Therefore, the edge flame stabilization mechanism under turbulence would be summarized with more
details. Premixing fuel with air in a jet pipe is another interesting topic. How would the flame base structures be and how would the flow fields vary? What would the influence of premixing be? What will the lean and rich branches distribute? These experiments will reveal the underlying physics.

7.2.3 Simulations of 3D lifted jet flames with high Re numbers and transitional processes

2D and 3D flows are qualitatively different, 3D turbulence dynamics more effectively aid our understanding of flame-turbulence interactions. Current simulations in the present research work are only 2D and use low Re numbers in DNS methods. The 3D simulations with an appropriate Re such as 4000~5000 which represents the flame base fluctuation is desirable for future work. Using the 3D simulations, we can find how the flame base structures look in 3D and we can determine flame base characteristics, such as, scalar dissipation rates, strain rates, flame propagation speed, and so forth.

Several different chemistry mechanisms should also be applied and compared here such as detailed and simplified hydrogen air and methane air reactions. It will not only reveal more information about the stability mechanisms but also provide hints for modeling with the LES or RANS methods.

Simulating the phenomena of lifted jet flame reattachment and blowout and comparing the results with experimental outcomes, will provide additional information.
7.2.4 Investigation of flame stability and flame Interactions with multiple fuel injections

In industrial applications, Fuel is usually injected into a high temperate zone. Several different injection positions with time delays may be involved. This flame stability, as well as considering low pollutions, is a very important topic in the flame stability research area. Simulations using the RANS and DNS methods are expected to provide much valuable information to help us design the industrial combustors better, which maintain better combustion stability and lower emission pollutants.
References


Appendices
Appendix A: Hydrogen Air 48-Step Detailed Reaction Mechanism

The table summarizes the detailed mechanism by Chen (1995), which was used as a starting point for the development of the four-step reaction mechanism used in Chapter 4. The mechanism is presented in terms of its forward and backward rates indicated separately.

<table>
<thead>
<tr>
<th>Nr.</th>
<th>Reaction</th>
<th>$A$ cm$^3$ sec$^{-1}$ K$^{-1}$ mole$^{-1}$</th>
<th>$n$</th>
<th>$E$ kcal/mole</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$H + O_2 \rightarrow OH + O$</td>
<td>$1.00 \times 10^{-6}$</td>
<td>0.00</td>
<td>16,800.0</td>
</tr>
<tr>
<td>2</td>
<td>$OH + M \rightarrow OH + H$</td>
<td>$1.50 \times 10^{-11}$</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>$O + H \rightarrow OH + H$</td>
<td>$5.00 \times 10^{-6}$</td>
<td>0.00</td>
<td>2.67</td>
</tr>
<tr>
<td>4</td>
<td>$O + H_2 \rightarrow OH + H$</td>
<td>$1.22 \times 10^{-10}$</td>
<td>0.00</td>
<td>4.378</td>
</tr>
<tr>
<td>5</td>
<td>$OH + H_2 \rightarrow H_2O + H$</td>
<td>$1.00 \times 10^{-12}$</td>
<td>1.60</td>
<td>3,296.3</td>
</tr>
<tr>
<td>6</td>
<td>$H_2O + H \rightarrow OH + H_2$</td>
<td>$1.31 \times 10^{-12}$</td>
<td>1.60</td>
<td>18,374.1</td>
</tr>
<tr>
<td>7</td>
<td>$2OH = O_2 + H_2O$</td>
<td>$1.50 \times 10^{-12}$</td>
<td>1.14</td>
<td>100.4</td>
</tr>
<tr>
<td>8</td>
<td>$O + H_2O \rightarrow OH + H_2O$</td>
<td>$1.47 \times 10^{-15}$</td>
<td>1.14</td>
<td>14,959.9</td>
</tr>
<tr>
<td>9</td>
<td>$O_3 + H + M \rightarrow H_2O_2 + M$</td>
<td>$3.30 \times 10^{-8}$</td>
<td>-0.80</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>$HO_2 + M \rightarrow O_3 + H + M$</td>
<td>$3.19 \times 10^{-16}$</td>
<td>-0.80</td>
<td>46,693.3</td>
</tr>
<tr>
<td>11</td>
<td>$H + HO_2 \rightarrow 2OH$</td>
<td>$1.50 \times 10^{-14}$</td>
<td>0.00</td>
<td>1,004.0</td>
</tr>
<tr>
<td>12</td>
<td>$H + HO_2 \rightarrow H_2O + O_2$</td>
<td>$1.50 \times 10^{-14}$</td>
<td>0.00</td>
<td>609.1</td>
</tr>
<tr>
<td>13</td>
<td>$OH + HO_2 \rightarrow H_2O + O_2$</td>
<td>$6.00 \times 10^{-14}$</td>
<td>0.00</td>
<td>0.0</td>
</tr>
<tr>
<td>14</td>
<td>$H + HO_2 \rightarrow H_2O + O_2$</td>
<td>$1.00 \times 10^{-14}$</td>
<td>0.00</td>
<td>1,723.8</td>
</tr>
<tr>
<td>15</td>
<td>$HO_2 + O + KO + OH$</td>
<td>$1.80 \times 10^{-11}$</td>
<td>0.00</td>
<td>-406.3</td>
</tr>
<tr>
<td>16</td>
<td>$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$</td>
<td>$1.50 \times 10^{-11}$</td>
<td>0.00</td>
<td>-1,242.0</td>
</tr>
<tr>
<td>17</td>
<td>$OH + OH + M \rightarrow H_2O_2 + M$</td>
<td>$2.50 \times 10^{-10}$</td>
<td>-2.00</td>
<td>0.0</td>
</tr>
<tr>
<td>18</td>
<td>$H_2O_2 + M \rightarrow OH + OH + M$</td>
<td>$1.69 \times 10^{-10}$</td>
<td>-2.00</td>
<td>48,348.0</td>
</tr>
<tr>
<td>19</td>
<td>$H_2O_2 + H \rightarrow H_2O + OH$</td>
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<td>0.00</td>
<td>1,581.0</td>
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<td>20</td>
<td>$H_2O_2 + OH + H_2O + OH_2$</td>
<td>$5.00 \times 10^{-12}$</td>
<td>0.00</td>
<td>1,003.8</td>
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<tr>
<td>21</td>
<td>$H_2O_2 + OH + H_2O + OH_2$</td>
<td>$1.00 \times 10^{-11}$</td>
<td>0.00</td>
<td>32,206.0</td>
</tr>
<tr>
<td>22</td>
<td>$H + M \rightarrow H_2 + O$</td>
<td>$1.80 \times 10^{-12}$</td>
<td>-1.00</td>
<td>0.0</td>
</tr>
<tr>
<td>23</td>
<td>$OH + H \rightarrow M \rightarrow H_2 + O$</td>
<td>$2.00 \times 10^{-11}$</td>
<td>-2.00</td>
<td>0.0</td>
</tr>
<tr>
<td>24</td>
<td>$O + O + M \rightarrow O_2 + M$</td>
<td>$2.90 \times 10^{-11}$</td>
<td>-1.00</td>
<td>0.0</td>
</tr>
<tr>
<td>25</td>
<td>$H_2O_2 + H \rightarrow H_2 + HO_2$</td>
<td>$4.790 \times 10^{-10}$</td>
<td>0.00</td>
<td>7,945.8</td>
</tr>
<tr>
<td>26</td>
<td>$OH + O \rightarrow M \rightarrow H_2 + O$</td>
<td>$1.00 \times 10^{-10}$</td>
<td>0.00</td>
<td>47,780.0</td>
</tr>
<tr>
<td>27</td>
<td>$H_2 + O \rightarrow M \rightarrow H_2 + O$</td>
<td>$1.70 \times 10^{-10}$</td>
<td>0.00</td>
<td>47,780.0</td>
</tr>
<tr>
<td>28</td>
<td>$OH + O \rightarrow M \rightarrow OH + OH_2$</td>
<td>$6.20 \times 10^{-10}$</td>
<td>-0.60</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Note: The table includes reactions for Nitrogen Chemistry.
Appendix B: RANS Simulation Settings in ANSYS-CFX

Appendix B summarizes the steps used to set-up the lifted jet computations in Chapter 6 with the CFX commercial CFD software.

B.1 Geometry and mesh resolution controls in ANSYS-Workbench

ANSYS-workbench is used to draw the simulation objective geometry and generate the 3D meshes. Point spacing control is used to refine the flame zone and flame edge zone mesh length scales. The software graphical user interface (GUI) is shown in Figure B.1.

![Figure B.1 Simulation domain and mesh resolution controls using Ansys-workbench](image-url)
B.2 Combustion and flow model settings in CFX-Pre

The combustion and flow models are set in the fluid model menu in CFX-Pre and the GUI is shown in Figure B.2. The set-up indicates that the k-ε model is used for turbulence closure and the eddy dissipation model (EDM) is used for combustion closure. In the EDM model, the following parameters are used in the indicated run. The chemical time scale, which corresponds to the variable $\tau_c$ in Chapter 6 is selected with a value of 0.0005 s. The extinction temperature, which is used to turn on or off chemistry, is set at 600 K. The mixing rate limit, which is the maximum allowed value of the local turbulent mixing rate, is set at 300 s$^{-1}$. The eddy dissipation model coefficient, $A$, is chosen here as 5.7; however, different values are adopted for this constant as discussed in Chapter 6.
Figure B.2 Combustion and flow models settings in CFX-Pre
B.3 New variables and quantitative definitions in CFX-Post

In the menus of variables and quantifies in CFX-Post, new variables can be defined and output directly in CFX-post. Quantitative are defined as expressions, and then connected to customized variables. One example is shown in Figure B.3.

**Figure B.3** New variable definitions and output in CFX-Post