THE UNIVERSITY OF OKLAHOMA

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# EFFECTS OF ELLIPTICAL BURNER GEOMETRY ON PARTIALLY PREMIXED GAS JET FLAMES IN QUIESCENT SURROUNDINGS

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By

Benjamin Baird

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## EFFECTS OF ELLIPTICAL BURNER GEOMETRY ON PARTIALLY PREMIXED GAS JET FLAMES IN QUIESCENT SURROUNDINGS

#### A DISSERTATION APPROVED FOR

#### THE SCHOOL OF AEROSPACE AND MECHANICAL ENGINEERING

 $\mathbf{B}\mathbf{Y}$ 

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# Chapter 5: Flame Structure

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## NOMENCLATURE

## English Symbols

ai	Collider species experimental constants
A <sub>21</sub>	Einstein spontaneous emission
	coefficient
A <sub>o</sub>	Avogadro's number,
A/F	Air to Fuel Ratio
С	Experimental constant
$\ell$	Distance from flame to pyrheliometer
lseg	Length of imaged probe laser segment
	(Rayleigh)
Δl	Length of the probe laser beam in the
	probe region (OH LIF)
x	Number of carbon atoms in fuel
EI	Emission index
F	Radiative fraction
h	Plank's constant
Ī	Incident probe laser intensity (Rayleigh)
Īr	Probe laser intensity (OH LIF)
I.	Intensity of Rayleigh Scattering
K	Rayleigh overall scattering factor
LHV	Lower heating value of the fuel
M	Molecular weight
m	Mass flow rate
n <sub>e</sub>	Number of molecules (OH LIF)
P <sub>acc</sub>	Gas pressure
$\Omega_{\rm s}$	Ouenching coefficient (OH LIF)
	Quenching rate of OH
R R	Corrected measured radiative flux
R	Gas constant of the gas
Re	Reynolds number based on cold jet
ite	conditions
Т	Gas temperature
i gas V	Frequency of the probe laser (OH LIF)
v ge	requency of the prove faser (off Eff.)
Greek Symbols	
$\sigma_{re}$	Absorption cross section of OH
σ	Collider species experimental constant
$-Q_{\infty}$	
2	(UH LIF)
$\mu_{ m ge}$	Boltzman traction of excited OH
	molecules
<u>()</u>	Solid angle of the collection optics

$\left(\frac{d\sigma}{d\Omega}\right)_{eff}$	Effective Rayleigh differential
	crossection of the gas
$\eta_{ m T}$	Combined transmission efficiency of the optics of the system (OH LIF)
$\eta_{ m D}$	Detection efficiency of the camera (OH LIF)
Φ	Equivalence ratio before leaving burner
χ	Mole fraction

Actual conditions (A/F)
Point of transition from laminar to turbulent (Re)
Based on effective diameter of burner
Collection efficiency of the detection optics (OH LIF)
Species i
Radiative flux incident on pyrheliometer
Property of the fuel air mixture
Hydroxide radical
Calibration constant of the collection optics (Rayleigh)
Stoichiometric (A/F)
Stern-Volmer coefficient

#### ABSTRACT

There is much work being done to improve the performance of combustion systems, both in increasing the efficiency of combustion and in reducing harmful products of combustion. One way of controlling the combustion process is through the so-called 'passive controls.' These methods involve changes to the geometry or initial conditions of the system. This affects such properties as air/fuel mixing rate and temperature profiles of the flame, both of which can have a great effect on the products of the flame.

This study is the investigation of the effect of elliptical nozzle burner geometry and partial premixing, both 'passive control' methods, on a hydrogen/hydrocarbon flame. Both laminar and turbulent flames for circular, 3:1, and 4:1 aspect ratio (AR) elliptical burners are considered. The amount of air mixed with the fuel is varied from fuel-lean premixed flames to fuel-rich partially premixed The work includes measurements of flame stability, global pollutant flames. emissions, flame radiation, and flame structure for the differing burner types and fuel conditions. Special emphasis is placed on the near-burner region. Experimentally, both conventional (IR absorption, chemiluminecent, and polarographic emission analysis,) and advanced (laser induced fluorescence, planar laser induced fluorescence, Laser Doppler Velocimetry (LDV), Rayleigh scattering) diagnostic techniques are used. Numerically, simulations of 3-dimensional laminar and turbulent reacting flow are conducted. These simulations are run with reduced chemical kinetics and with a Reynolds Stress Model (RSM) for the turbulence modeling.

It was found that the laminar flames were similar in appearance and overall flame length for the 3:1 AR elliptical and the circular burner. The laminar 4:1 AR elliptical burner flame split into two sub-flames along the burner major axis. This splitting had the effect of greatly shortening the 4:1 AR elliptical burner flame to have an overall flame length about half of that of the circular and 3:1 AR elliptical burner flames. The length of all three burners flames increased with increasing burner exit equivalence ratio.

The blowout velocity for the three burners increased with increase in hydrogen mass fraction of the hydrogen/propane fuel mixture. For the rich premixed flames, the circular burner was the most stable, the 3:1 AR elliptical burner, was the least stable, and the 4:1 AR elliptical burner was intermediate to the two other burners. This order of stability was due to two reasons. The elliptical burners have enhanced turbulence generation that lowers their stability when compared to the circular burner. The 4:1 AR elliptical burner had greater stability due to a greater velocity decay rate and wider OH reaction zones particularly in the region between the two jets.

The 3:1 AR elliptical and circular burners produced similar carbon monoxide and nitric oxide emission indexes over the range of equivalence ratios of 0.55 to 4.0, for laminar flames. The 4:1 AR elliptical burner produced greater CO and lower NO emission indexes than the other two burners for laminar flames. For all burners, an increase in the equivalence ratio tended to decrease the production of CO and increase the production of NO. For the turbulent flames, both the elliptical burners resulted in the production of more CO and less NO than the circular burner, with the difference between the elliptical and circular burner emission production being greater at an equivalence ratio of 2.0. The NO production is linked to the flame length and temperature level of the flames, while the CO production is a function of the fluid dynamics of the burners.

It was found that the results of this study would be that 4:1 AR elliptical burners with premixed flames have the primary benefit of having much shorter flames. This will allow much shorter combustor design and reduces the nitric oxide emissions. However, the reduction in length comes at the cost of a small loss of stability and an increase in carbon monoxide emission. With premixed flames, the elliptic burner with a 3:1 AR performed substantially similar to the circular burner with a loss of stability.
# **CHAPTER 1: INTRODUCTION**

#### **<u>1.1: Motivation</u>**

In the past few decades, there has been an emphasis on research into methods of combustion that increase efficiency while decreasing harmful emissions. These control methods can be grouped into two categories, namely, active and passive controls. Active controls include methods that modify the flame by applying some external influence on the combustion system. Examples include modification of the flame properties by acoustic forcing or by the use of electromagnetic fields. Passive controls involve changes in the initial conditions of the combustion system to adjust the flame dynamics. This is done by selection of fuel type, by premixing the fuel and oxidant, or by modifying the burner geometry. This study concerns the two passive control techniques of burner modification, specifically the use of elliptical burner geometry, and the use of fuel/air premixing. Considerable work has been done on cold-flow elliptic jets and diffusion flames produced by elliptical jets, but very little work has been done with elliptical premixed flames. The study of elliptical burner premixed flames could be of great use, considering the current push for emission reduction using ultra-lean-combustor (ULC) designs.

# **1.2: Objectives**

The purpose of the study is to gain a better understanding of the mixing and combustion processes in premixed and partially premixed flames with elliptical exit burners. Of particular interest are the effects of ellipticity on the stability, thermochemical structure, emissions and radical concentrations in premixed and partially premixed gas jet flames. The study covers the following for the conditions of varying aspect ratio (circular, 3:1, and 4:1) and varying levels of partial premixing (0.55, 1.0, 2.0, and 4.0 equivalence ratio):

- Measurement of flame stability (blowout velocity for a given equivalence ratio)
- Description of flame appearance
- Flame length measurements
- Measurement of emission indices (CO<sub>2</sub>, CO, and NO)
- Measurement and characterization of flame radiation
- Measurements of mean velocity and turbulent fluctuation
- Measurement of temperature profiles at the near-burner, midflame, and far-flame
- Measurement of concentration profiles (CO<sub>2</sub>, CO, O<sub>2</sub> and NO) at the near-burner, midflame, and far-flame
- LIF measurement of OH concentrations
- Numerical simulation of turbulent premixed flames from elliptic exit burners

# 1.3: Project Impact

First, one of the important, up-and-coming methods for reducing emissions from power generating devices is the ultra-lean-combustor (ULC) concept. ULC burners are designed to run at very high level of premixedness, often near the flammability limits. This very lean operation reduces the temperature of the flame, thereby reducing the nitric oxide production of the burner greatly. Reducing the temperature also allows a greater efficiency of the combustor (through a reduction of heat losses) and allows the use of lower tolerance materials for the combustor design, reducing the operational cost. Using ULC to lower emissions and increased efficiency comes with a cost in that ULC burners tend to be subject to flame oscillations and frequent blowout, both undesirable traits. This is because lean flames are very sensitive to inlet conditions, either through fluctuations in equivalence ratio or inlet velocity, or through acoustic disturbances. Elliptic burner geometries, with their unique flow properties, may be useful in attenuating these changes.

Premixed flames are also commonly found in industrial and residential applications, from household cooking to large smelting furnaces. Given the breadth and range of applications of premixed flames a small increase in efficiency or other potential benefits could produce large effects.

Finally, the use of elliptical burners with premixed flames will help shed light on some fundamental flame properties. The regions of high and low flame curvature generated by the burner will be ideal for expanding knowledge about how stretching affects a flame, particularly in the sense of radical focusing and defocusing.

## **<u>1.4: Dissertation Overview</u>**

Chapter 2: Literature survey of non-circular and premixed flames, development of basic theories of measurement.

Chapter 3: Description of experimental apparatus and procedure.

Chapter 4: Presentation of results involving global flame properties, such as stability, flame appearance, flame length, emission indexes, and radiation parameters.

Chapter 5: Presentation of results involving internal structure of the flame, such as the flame flow field (from PDPA and schlieren images), temperature profiles, concentration profiles of stable species (CO,  $CO_2$ ,  $O_2$ , and unburned fuel), and concentration profiles of intermediate species of combustion (OH).

Chapter 6: Presentation of computational results. Includes description of mathematical model, grid parameters, grid independence measurements, and comparison of computational results with experimental.

Chapter 7: Conclusions and recommendations for future studies.

### **CHAPTER 2: LITERATURE REVIEW AND BACKGROUND THEORY**

# 2.1: Background\Previous Work

**2.1.1 Elliptical Jets/Elliptical Flames:** Crighton (1973) did the early work on elliptic non-reactive jets by performing an analytical study of non-reactive high aspect ratio elliptical jets. He determined that, from a temporal perspective, elliptic jets were stable. Spatially, though, he found that disturbances parallel to the major axis of the jet have small growth rates while those parallel to the minor axis have large growth rates. This analysis hinted at a phenomenon that would later be called 'axis switching'.

In their work, Ho and Gutmark (1987), defined the axis switching distance as the distance from the outlet of a non-circular nozzle where the jet cross-section changed its orientation, i.e., the minor axis became the major axis and vice versa. This is caused by a differential growth rate between the minor and major axis. In an elliptical jet, axis switching occurs several times along the streamwise direction of the jet. In their work with a 2:1 aspect ratio (major axis/minor axis) nozzle, they found on the major axis plane that the shear layer of the jet spread into the potential core while on the minor axis, the shear layer spread out into the surrounding fluid. They reported that mass entrainment was increased with an elliptical jet compared to a circular jet. This increase was attributed to the motion of the vortices developed by the jet.

In their study of elliptical jets of aspect ratios of 2:1 and 4:1, Hussain and Husain (1989) noted similar results. In addition, they reported that in the 4:1 nozzle, axis switching was replaced by a bifurcation of the jet. This bifurcation was characterized by the jet, instead of switching axes, spliting into two vortical structures. These vortices

form on either side of the major axis. Bifurcation was not seen with the 2:1 aspect ratio nozzle.

Gollahalli et al. (1992) performed a study on non-circular diffusion flames. They studied the liftoff and reattachment behavior of elliptical flames, and the temperature, emission, and velocity profiles produced by these flames. They found that the flame stability was lower, temperature and nitric oxide concentration were increased in the mid range, and soot production was reduced in elliptical flames. It was also found that the flow characteristics of non-reacting jets were applicable to reacting jets.

Miller et al. (1995) did a computational study of non-circular jets that included 1:1 and 2:1 aspect ratio (AR) elliptical, rectangular, and triangular jets. With a 'Flux Corrected Transport' finite difference algorithm they performed velocity and entrainment studies of non-circular nozzles. They were able to capture the development of the vortex structure as reported by Ho and Gutmark and Hussain and Husain.

Kamal (1995) performed a study on the effect of the jet exit Reynolds number, nozzle exit size, and nozzle aspect ratio on turbulent diffusion flames. In the study, he found that combusting elliptical jets entrain more air, produce more  $CO_2$ , have higher peak temperatures, generate less soot, emitted less radiation, and were less stable than circular jets. He also found that the advantages of ellipticity decreased with the increase of the jet Reynolds number or an increase in the burner size.

Papanikolaou and Wierzba (2001) did a study on elliptical burners in coflow. They tested a range of aspect ratios from 1.29 to 1.60 with methane diffusion flames focusing on the stability aspects of the burners. They found that the ellipticity of the burner of the tested range did not have a large affect on the blowout behavior but

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ellipticity did affect the stability of attached flames significantly. They observed that the presence of the flame retarded jet spread, delayed axis-switching of the jet, and decreased the velocity decay along the centerline of the jet. The presence of the flame also suppressed the turbulence intensity.

Gollahalli and Pardivalla (2002) preformed a study of diffusion flames in crossflow using a 3:1 AR elliptical burner and a circular burner of equivalent exit area using propane as the fuel. It was found that the 3:1 AR elliptical burner with major axis perpendicular to the crossflow had stable flames at a higher burner exit jet velocity and produced longer flames than the circular burner. With the minor axis set perpendicular to the crossflow, the 3:1 AR elliptical burner was stable at a lower burner jet exit velocity and exhibited shorter flames. The elliptical burners tended to produce less CO and more NO than the circular burner.

**2.1.2 Premixed/Partially Premixed Flames:** Mueller, et. al. (1995) studied the interaction of vortexes with premixed flames. This was done by the production of a vortex of unburned reactants that was produced to impinge on a 2-dimensional flame propagating though the premixed fuel mixture. Through the use of particle-imaging velocimetry and OH laser induced fluorescence, they determined that the experimental measurements had significant deviation from predictions based on steady counter flow experimental results.

Echekki and Chen (1996) performed 'direct numerical simulations' of wrinkled premixed methane/air flames to determine the effects of flame curvature on flame structure. In this study, they found that flame curvature had a greater effect on fast

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reacting and highly diffusive species compared to slower species. For example, they found that  $H_2$  and H molecules were increased in areas convex and depleted in areas concave to the reaction products side of the flame. This focusing and defocusing of species had significant effects on the flame. The enhanced hydrogen concentrations increased CH<sub>4</sub> reactions, the heat release rate, and the flame propagation speed. Slower reacting/diffusing species, such as CO, did not exhibit focusing behavior but did have some correlation with the flame stretch, with positive stretch depleting and negative stretch increasing concentration.

Helenbrook et al. (1996) modeled the propagation of an initially planar premixed flame through a channel that contained a series of vortices. From the results of the model, they determined that stretching in the flame caused by the vortices caused a decrease in the mean burning velocity of the flame but in order for the effect to be significant, the vortexes had to have a size on the same order as the flame thickness. Interestingly, when the computational results were compared to experimental results, there were significant differences. Specifically, pockets of unburned reactants were seen to develop in the flame front in the model, but these pockets of unburned gas were not seen in experimental results.

With an experimental study of spherical hydrogen/air laminar premixed flames of fuel equivalence ratios ranging from 0.3 to 5.0, Aung et al. (1997), made several important conclusions. Like Helenbrook et al., they concluded that flame stretch had a significant effect on the burning velocity. They also concluded that the stability characteristics of the flame at fuel rich and fuel lean conditions were determined primarily by the high diffusion rate of hydrogen compared to oxygen. At intermediate equivalence ratios, however, stability was found to be determined by bulk heat and mass diffusion as well as the reactivity of the radicals produced by the flame.

Najm and Wyckoff (1997) performed a numerical study of a 2-D counter rotating vortex pair interacting with a premixed stoichimetric methane-air flame. In the study, they found that the thermal thickness of the flame became narrower in regions of positive flame strain (where a differential area of the flame increases with time) and wider in regions of negative flame strain (where the differential area reduces with time). They also concluded that focusing and defocusing of combustion intermediates occurred at curvatures and that this focusing/defocusing was of intensity sufficient to change the extinction properties of the flame.

Røkke et al. (1994) studied partially premixed lifted flames established over a straight tube in quiescent air. The fuel mass fraction of the jet was varied from 1.0 to 0.15. The flames studied were of a large scale with flame lengths approaching 2.5 m. The authors reported that liftoff height was inversely proportional to the square root of the mass fraction of the fuel in the partially premixed jet. They also reported that the flame height decreased with an increase in the air-fuel ratio. They found that an increase of air entrainment into the fuel stream increased the NO<sub>x</sub> production of the flame.

Gore and Zhan (1996) performed an experimental analysis of the visible flame height, global radiative heat loss, and emissions of fuel rich laminar partially premixed flames of methane and air in a co-flow stream of air. They reported that increasing the air/fuel ratio in the fuel jet caused a decrease in the visible flame height with the color of the flame changing from a highly luminous yellow color to a less luminous blue. The radiative heat loss initially decreased with the increase of air-fuel ratio, but eventually approached a constant value. Also, the CO concentration decreased and the  $CO_2$  and  $H_2O$  concentrations increased as the flame became more fuel lean.

Lee et al. (1997) studied the effects of varying the degree of premixing of partially premixed turbulent flames by creating a special coaxial burner arrangement. In their burner arrangement, they introduced fuel into a co-flowing air stream. A flame was then established downstream. The extent of premixing was controlled by changing the relative positions of the fuel and air streams and by varying the fuel to air jet velocity ratio. It was found that the more complete the fuel and air mixing, the shorter the flame height and the lower the radiative emission of the flame.

Choi and Puri (2000) performed an experimental study of partially premixed flames of methane and air for a range of equivalence ratios of 1.24 to 2.1 using a slot burner. Their focus was on curvature effects on premixed flames, particularly at the tip of the flames.. They reported two reaction zones in the flame, an inner premixed and an outer non-premixed reaction zone. They also reported that the effective flame speed in curved regions was greater than that seen in non-curved regions of the flame.

Wehrmeyer et al. (2001) performed a numerical and experimental study of the effects of flame curvature on premixed propane/air and hydrogen/air flames. Numerically, they found that for propane flames, that when the flame was curved concave towards the unburned fuel/air stream, increasing curvature increased the temperature of the flame due to focusing of the heat produced by combustion. For hydrogen/air flames, for the same condition of the flame curved concave towards the unburned fuel/air stream, the temperature decreased with increasing curvature due to to

defocusing caused by diffusional mass transfer of hydrogen. Their experimental study confirmed the results seen with computational predictions.

Hariharan (2004) researched the effect of coflow air on elliptic premixed propane/hydrogen/air flames with aspect ratios of 3:1 and 4:1 and on circular burner flames. Hariharan used a 40% by mass mixture of hydrogen in propane and studied flames of equivalence ratio of 1.0 to 4.0. The flames were turbulent. In the study, he reported that for quiescent conditions, the 3:1 AR elliptical burner had a higher blowout velocity than the circular burner and the 4:1 AR elliptical burner, but the difference was very small. The circular burner had the longest flames, followed by the 3:1 AR elliptical burner with the 4:1 AR elliptical burner having the lowest flame length, and that the circular burner produced greater CO and NO emissions than the elliptical burners.

From this review of the literature, several points are clear. First, much work has been done on cold elliptical jets and from this work it has been found that elliptical jets increase the entrainment of a jet by the development of unstable vortices and the by the phenomenon of axis switching, both of which act to 'pump' surrounding air into the jet. Also, it is seen that much work has been done on diffusion flames produced by burning elliptical jets with detailed flame stability, flame length, radiative heat loss fraction, and emission studies having been reported. However, little work has been done on the effects of non-circular burner geometries on premixed and partially premixed flames. The work done so far on geometry effects has focused on the variation of fuel and co-flow air tube positions and opposed flow setups. From the existing premixed and partially premixed flame literature, several phenomena have been identified that may have significant effects on premixed elliptical flames. First, it has been found that intermediate radicals in the flame can be focused and defocused depending on the amount of curvature of the flame front. Since the elliptical flame has regions of high (near the ends of the major axis) and low (near the ends of the minor axis) curvature and regions of high and low flame strain rates (due to differential growth rates that result in axis switching), it is of interest to investigate how these regions interact with each other.

#### **CHAPTER 3: EXPERIMENTAL SETUP AND PROCEDURE**

#### 3.1: Experimental Facility

**3.1.1 Combustion Chamber:** The nozzle burners were located in a vertical steel combustion chamber (Fig. 3.1.1) of 76 cm by 76 cm cross section and 147 cm height from the bottom of the chamber to the beginning of the exhaust contraction at the top of the chamber. Three of the walls were fitted with Pyrex plate glass windows (25.4 cm by 131 cm) and the fourth wall was fitted with a metal sheet with a machined 1.4 cm by 127 cm vertical slot centered horizontally for instrument access. The top of the combustion chamber was open to atmosphere pressure through an exhaust duct that vented to the exterior of the laboratory. The ambient pressure of the lab was maintained slightly (0.17 mm Hg) above atmospheric pressure to ensure a positive draft inside the test chamber in order to reduce the escape of products of combustion into the main laboratory facility. A 16 cm diameter opening in the base plate of the test chamber provided for incoming fresh air into the chamber. A 36 cm diameter flow diverter plate was installed at a height of 4 cm above the chamber base plate opening to diffuse the incoming airflow to create quasi-quiescent air conditions within the chamber.

**3.1.2 Burner and Fuel Delivery System:** The fuel used in this study consisted of mixtures of commercial quality propane and hydrogen with component compositions given in Table 3.1. A mixture of propane and hydrogen was used to create burner-stabilized flames with high jet exit velocity (Reynolds number) to study turbulence effects. Propane fuel-only premixed flames tended to liftoff at very low jet exit velocities

and introduced additional complexities due to liftoff, and consequently made the determination of the effects attributable to burner geometry difficult. Thus, the addition of hydrogen was used to anchor the flame to the burner by greatly increasing the liftoff velocity of the flame. More details regarding this behavior will be given in Section 4.1.

The propane, hydrogen, and air were supplied at a pressure of 138 kPa from highpressure cylinders. The volume flow rates of the propane, hydrogen, and air were controlled with calibrated rotameters and needle valves. The propane and hydrogen components were mixed with a simple y-connection. This propane/hydrogen mixture and air were combined inside an annular mixing device (Fig 3.1.2a).

This mixing device consisted of an off-the-shelf <sup>1</sup>/<sub>4</sub> inch diameter (6.4 mm) copper inner tube surrounded by a <sup>1</sup>/<sub>2</sub> inch diameter (12.7 mm) copper outer tube. Major dimensions of the mixing device are given in Fig. 3.1.2.a. There was 15.2 cm of mixing length in the mixing device. The typically higher volume flow rate of air (compared to the propane/hydrogen mixture) was injected in the center tube in order to entrain the propane/hydrogen mixture that was supplied to the concentric outer chamber.

The length of the mixing device and tubing connecting the mixing chamber to the burner assembly (Fig. 3.1.2b) combined with the length of tubing connecting the mixing chamber to the burner was sufficiently long (greater than 250 diameters) to ensure a homogenous mixture of air and fuel through the natural mixing processes of flow through a tube. In order to reduce the potential of flashback, a sintered metal filter element of pore size 15  $\mu$ m was used to prevent a flame from propagating into the fuel supply line upstream of the fuel-air mixing device.

From the mixing chamber, the fuel/air mixture was passed to the burner assembly through a length of <sup>1</sup>/<sub>4</sub> inch copper tubing. To allow movement of the burner assembly, a length of flexible tubing was placed in the path of the copper tubing connecting the mixing chamber to the burner assembly. Upstream of the flexible tubing a pressure tap was placed to monitor line pressure.

The burners of the study were mounted at the end of a <sup>1</sup>/<sub>2</sub> inch iron pipe of length 30.5 cm. The fuel/air mixture was introduced into the other end of this pipe with a <sup>1</sup>/<sub>4</sub> to <sup>1</sup>/<sub>2</sub> inch fitting. The use of the iron pipe served two purposes; settling of the fuel/air mixture flow through the velocity drop with the rapid expansion from a <sup>1</sup>/<sub>4</sub> to <sup>1</sup>/<sub>2</sub> diameter and it gave a convenient mounting point for the burner. The entire burner assembly was attached to a 2-D linear traverse mechanism to allow adjustment of the burner height and horizontal position of the burner. This was done to facilitate the development of radial profiles for the flame.

Three burner geometries were considered in this study (Figs. 3.1.3a and b and Table 3.1): a circular nozzle of exit inside diameter 2.0 mm, a 3:1 aspect ratio elliptical nozzle of exit inside dimensions 3.4 mm for the major axis by 1.2 mm for the minor axis, and a 4:1 aspect ratio elliptical nozzle with exit inside dimensions of 4.0 mm for the major axis and a 1.0 mm for the minor axis. These dimensions were determined to give equal outlet areas. In this study, the equivalent diameter was defined to be the diameter of a circle with area equal to the outlet area of the elliptical burner.

Figures 3.1.4a through c show the radial mean axial cold jet velocity distribution at 1 mm above the burner exit for the three burners of this study for a jet exit velocity of 20 m/s. The three burners gave a reasonably constant exit gas velocity across the entire outlet area.

#### 3.2: Instrumentation

**3.2.1 Flame Visualization:** Images of the flame were recorded using a digital video camera (JVC Model GR-DVL815U). In order to obtain these images, digital video data were recorded under constant lighting conditions with a dark background using a 1/100 second camera shutter speed. The image plane was focused on the plane that passes through the center of the nozzle burner. To calibrate for length, images of a scale placed on that plane were used.

Images were taken from a view perpendicular to both the major and minor axis planes of the elliptical flames. Ten images per flame condition were taken at arbitrary time intervals between images and the resultant image flame lengths were averaged. For the purposes of this study, with the low luminosity flames characteristic of premixed combustion, the flame length was determined by measuring the distance from the top of the burner to the farthest point that had a noticeable increase in brightness from the background of the image. This was done by loading the images in to the Adobe Photoshop image processing software package. Given the low contrast between the background and the outer flame of the premixed flames, the contrast and brightness of the images were increased 20% and 30% respectively. The number of pixels from the base of the flame to the farthest point of brightness of the flame, determined by an adjusted brightness level of 10% above the background intensity, was counted and recorded. This pixel count was converted into a length scale using the scale image as a calibration reference. Although this was a somewhat subjective method of flame length measurement, for relative comparisons of the effects of the burner geometry and jet exit equivalence ratio on flame length, it was reasonable and reproducible.

**3.2.2 Schlieren Imaging:** Schlieren imaging is a commonly used experimental method that can detect gradients of concentration and/or temperature in a region of space. Schlieren imaging works on the principle of variation in the refractive index due to density gradients. This variation deflects light passing through a test region creating an image that consists of dark and light areas. Dark areas correspond to regions of high refractive index gradients while light areas are regions of small gradients.

For the current study, grayscale schlieren images were taken using the method of knife-edge schlieren (Fig. 3.2.1). A 250W quartz halogen continuous light source (Cuda Products Corp, Model 1-1250) was routed through a high throughput fiber optic cable to a pinhole of diameter 1.0 mm. This point source of light was then colliminated/decolliminated using a matched pair of lenses of focal length and diameter 300 mm and 66 mm respectively. The colliminated light beam was passed through the region of testing. At the focal point of the decolliminating lens, a knife-edge was used for gradient enhancement. The resultant image after use of the knife edge was focused on the high speed camera with a Cosmicar/Pentax TV zoom lens. Images were recorded using a high-speed camera (MotionScope 2000 S camera from RedLake MASD) at a shutter speed of 1/20000 second. To observe changes along the axial length of the flame, images were taken at multiple heights above the burner.

**3.2.3 Temperature Profiles:** Due to the large percentage of hydrogen in the premixed flames of the study, conventional thermocouple measurements were fraught with difficulty. Normally, platinum/rhodium thermocouples (type S, R, etc) are used for

diffusion flame studies, but they are unsuitable for the premixed flames of this study due to a maximum service rating of 1768 °C. Tungsten/rhenium thermocouples have a higher melting point (maximum service rating of 2320 °C), but tend to oxidize rapidly at high temperatures. Due to premixing, there was oxygen throughout the flame of the current study. Temperature profiles were therefore measured using the well-established (Dibble and Hollenback (1981), Wolfrum (1998), Meier et al. (2000), Watson et al., (2000), Kearney et al. (2003)) mechanism of Rayleigh scattering.

Rayleigh scattering gives a non-intrusive, relatively accurate means of measuring temperature in a gas. Rayleigh scattering is the result of elastic interactions between incident photons and the molecules that make up a gas. The magnitude of the scattering is dependent on the incident probe wavelength and power, gas composition, and gas number density. For the purposes of this study, the gas was considered as being primarily nitrogen throughout the flame. This was reasonable given that the premixing of the fuel and air results in a nearly 70% by volume N<sub>2</sub> content in the combusting jet. Making this assumption allows us to calculate the gas temperature using the ideal gas relation.

The Rayleigh probe beam (Figure 3.2.2) was created using the 355 nm output of a NdYAG laser (Spectra Physics GCR-250-10). The laser emission had a pulse width of <10 ns. The beam was guided by two, high efficiency, narrow bandwidth mirrors to a focusing lens. This lens focused the beam to a 0.5 mm beam diameter over the region of testing. The laser pulse power was monitored using a retro reflection of this focusing lens. After passing through the detection region, the probe beam was then sent to a beam dump.

The Rayleigh scattered radiation was collected at 90° to the incident beam path by a focusing lens of 32.4 mm diameter and a focal length of 60 mm. Using two mirrors the collected scattered radiation was folded 90° to convert the horizontal beam path to a vertical orientation for introduction into a spectrograph (Oriel Instruments MS257 Model 77700) equipped with a holographic grating (Oriel Instruments, Model 77740 1/4m Monochromator/Spectrograph Grating). In order to give good spatial and wavelength resolution, an inlet slit of 250 µm was used on the spectrograph. To detect the Rayleigh scattering and reject background noise, the spectrograph was set to a central wavelength of 355 nm.

The resultant filtered radiation was routed to and detected by an Intensified Charge Coupled Device (ICCD) camera (Princeton Instruments ICCD-576-G/RB-E). In order to further reduce background noise, the camera was gated to the 20 ns interval bracketing the incident laser pulse. Timing of the ICCD camera was achieved by triggering the image acquisition by an advance trigger signal from the GCR. This advance trigger occurs at a user adjustable interval before laser emission. The advance trigger to camera gate interval was adjusted using a Princeton Instruments Programmable Pulse Generator Model PG-200 to maximize the magnitude of the detected radiation. The scattered radiation was spatially resolved on the ICCD by the spectrograph.

Measurements of the Rayleigh scattering were made using the WinSpec software by taking a 12 pixel bin (corresponding to an integration length of 0.85 mm along the beam length) of every other 12 pixel region, giving 32 measurements per field of ICCD data. The field of view of the system allowed high-resolution temperature measurements, but multiple fields were required to collect the entire width of the flame. The flame was therefore scanned through the detection field with overlap between successive fields in order to ensure consistency in the data. Data were accumulated for 10 pulses per field. The collected data were then corrected for the ICCD camera dark field values, incident laser power fluctuations, and variations of sensitivity across the ICCD array. Temperature was derived from the data using the Rayleigh scattering intensity relation given by Dibble and Hollenbach (1981) which was given as:

$$I_{s} = C_{opt} I\Omega I_{seg} \frac{P_{gas} A_{o}}{R_{gas} T_{gas}} \left(\frac{d\sigma}{d\Omega}\right)_{eff} = \frac{KI}{T_{gas}} \left(\frac{d\sigma}{d\Omega}\right)_{eff}$$

(3.1) where  $I_s$  was the scattered intensity,

C<sub>opt</sub> was the calibration constant of the collection optics,

I was the incident probe laser intensity,

 $\Omega$  was the solid angle of the collection optics,

lseg was the length of the probe laser segment imaged on the detector,

Pgas was the gas pressure,

Ao was Avogadro's number,

R<sub>gas</sub> was the gas constant of the gas,

T<sub>gas</sub> was the gas temperature,

 $\left(\frac{d\sigma}{d\Omega}\right)_{eff}$  was the effective Rayleigh differential cross section of the gas

mixture, and

K was an overall Rayleigh scattering coefficient.

It is noted that, for the current experiments, many of the above factors were constant so, to simplify the scattering formulation, these constants were combined into an overall scattering coefficient, K. Using equation 3.1, K was developed by taking the

intensity of the Rayleigh scattering for atmospheric conditions (i.e. taken with no flame) and multiplying by the atmospheric temperature. For this study, the atmospheric data were repeated five times for 10 pulse accumulations. The atmospheric test was repeated prior to each flame test condition in order to track changes in laser intensity and camera sensitivity over the Rayleigh measurements.

**3.2.4 Velocity Profiles:** Gas jet velocity was measured using a Phase Doppler Particle Analyzer (PDPA) system produced by Aerometrics, Inc consisting of a transmitter (Model XMT-1100-5), receiver (Model RCV 2100-5), phase Doppler processor (Model PDP-3100-5), and motor controller (Model MCB-7100-3) operated by the PDPA v.P3.62 software. A PDPA operates by measuring the light scattered by particles in a flow to make a simultaneous measurement of particulate size and velocity. Velocity can be measured by the temporal variation of the scattered light. While particle sizing data collection was possible with the equipment, for the purposes of this study, only velocity data was taken, since the seed particle size was not of interest.

For this study, only the axial velocity component of the flowing gas was measured. Magnesium oxide with a particle size of approximately 1 µm was used for flow seeding. Magnesium oxide was chosen for its relatively high melting point (2300 °C) and ready availability. The seeding material was incorporated into the airline of the premixed flames due to the higher flow rate of air compared to the fuel for the flames of this study. A cyclone seeder was used to disperse the particles in the air. The PDPA receiver was located at a 150-degree angle from the transmitter (Fig. 3.2.3).

important PDPA settings are given in Table 3.2. Since the magnesium oxide particles were opaque, only reflective scattering was considered.

For profile measurements, the flame was scanned through the detection field with a stepper motor driven linear array. Centering of the PDPA measurement volume was done by the visual centering of the probe laser illuminated seed particles with the easily seen inner flame region ("bright blue"). This worked well for the near-burner and midflame, but had difficulty with the location of the exact center for the far-flame (due to lack of structure). However, a small variation in the position of the probe laser at the farflame should not affect results greatly due to the small variation of velocity magnitude at that region. The profile centerline was determined by finding the symmetric line of the generated profiles.

**3.2.5 Global Emissions** / **In-Flame Species Concentration Profiles:** Global emissions (Figure 3.2.4a) were taken with a Pyrex gas collection funnel placed over the flame so the total post combustion products are collected and mixed. A quartz sample probe of tip inner diameter of 0.5 mm and tip outer diameter of 1.8 mm increasing to a inner diameter of 4.9 mm and outer diameter of 7.1 mm was placed at the top end of the funnel to take a sample of the product gases.

In-flame species concentration profiles (CO<sub>2</sub>, CO, NO, and O<sub>2</sub>) (Figure 3.2.4b) were taken with a custom-made uncooled ceramic/quartz gas sample probe (Figure 3.2.4c). This probe consisted of a short length of ceramic tubing of inner diameter of 0.5 mm and outer diameter of 0.9 mm cemented with high temperature ceramic adhesive into a quartz holder. The quartz tube had inner and outer diameters of 4.9 mm and 7.1 mm

respectively. The probe was designed to withstand the high temperatures produced by this flame, which would tend to soften a plain quartz probe, plugging the inner diameter.

Gas samples for the in-flame concentration measurements were taken with the probe placed perpendicular to the flame centerline (as shown in Figure 3.2.4c, noting that the figure is an overhead view of the flame/probe configuration) at a position slightly short (~1 mm) of the centerline to account for the location of the sampling volume of the probe. In-flame concentration profiles were taken at the same positions along the flame as the temperature and velocity profile data to allow correlation of data.

Carbon dioxide and carbon monoxide concentrations were measured with a Non-Dispersive Infrared Analyzer (NDIR) (Rosemount Analytical Model 880A). Nitric oxide concentration was measured with a Chemiluminescence NO-NO<sub>2</sub>-NO<sub>x</sub> Analyzer (Thermo Environmental Instruments Model 42H). Oxygen concentration was measured with a polarographic sensor (MSA Catalyst Research MiniOX I).

For the global emissions, in order to correct for dilution of the product gases due to ambient air entrainment, an emission index was calculated following the method reported by Turns [14]:

$$EI_{i} = \left(\frac{\chi_{i}}{\chi_{co} + \chi_{co2}}\right) \left(\frac{xM_{i}}{M_{F}}\right)$$
3.1

where  $\chi_i$  was the mole fraction of the species of interest,

 $\chi_{CO}$  was the mole fraction of carbon monoxide,  $\chi_{CO2}$  was the mole fraction of carbon dioxide, x was the number of carbon atoms per mole of fuel, M<sub>i</sub> was the molecular weight of emission of interest,

M<sub>F</sub> was the molecular weight of the fuel.

Since the emission index is a ratio of concentration values, it was independent of dilution.

**3.2.6 Radiative Emissions:** Total Flame radiation was measured using a pyroheliometer (Hy-Cal Engineering Model P-8410-B-10-120-XC-400). This pyroheliometer had a detection angle of 150 degrees. The pyroheliometer had a linear output with a sensitivity of 28.4 ( $W/m^2$ )/mV. The pyroheliometer was located so that the entire flame was in the field of view and at a distance longer than 1.5 flame lengths to satisfy the inverse square law (Brzustowski, et al, (1975)). Output was collected using a computerized data acquisition system using a 1-second sample interval with a 1000 Hz sampling rate. The resultant 1000 data points were averaged, corrected for background radiation, and converted to a radiative fraction (F).

The radiative fraction was given by:

$$F = \frac{4\pi\ell^2 R_{\text{incident}}}{\dot{m}LHV_{\text{mixture}}}$$
 3.2

where  $\ell$  was the distance from the flame centerline to the pyrheliometer,

 $R_{incident}$  was the corrected measured radiative flux (W/m<sup>2</sup>),

LHV<sub>mixture</sub> was the lower heating value of the premixed gas mixture (J/kg), and

 $\dot{m}$  was the mass flow rate of fuel mixture (kg/s).

This gave the fraction of energy input to the burner that was released in the form of radiation.

The spectra of the radiation, Fig 3.2.5, were taken using a spectrometer (Oriel Instruments, MS257 Model 77700) with a holographic grating (Oriel Instruments, Model 77740 1/4m Monochromator/Spectrograph Grating). The scan was taken with a 2 nm step in the center wavelength for a range of 200 to 700 nm with the inlet and exit slits of the spectrometer set to produce a 2 nm band pass. A photomultiplier tube (Oriel Instruments, Model 77345) was used to get intensity data from the output of the spectrometer. Twenty data points were taken at equal intervals over a 2 second period for each wavelength step. This data were then averaged.

**3.2.7 LIF/PLIF Instrumentation:** Laser Induced Fluorescence (LIF) and Planar Laser Induced Fluorescence (PLIF) are well established techniques for measuring transient radical concentrations in flames (Daily (1977), Andresen et al. (1990), Roberts et al. (1992), Reisel et al. (1997), and Donbar et al. (2000)). Both operate on the principle of selective absorbsion and reemission of light by molecules.

In LIF/PLIF, a wavelength controlled narrowband light source (i.e. a tunable laser) is used to excite molecules of a species of interest to a higher energy level. After excitation, the excited molecules radiate the excess energy at known wavelengths. From the measured intensity of this emitted light, an estimate of the total number of molecules of the species of interest can be made. For this report, the method of LIF/PLIF was used for measuring the concentration of OH. OH was chosen because it is a good indicator of the intensity of combustion and also marks the oxygen side of the flame boundary. This can be used to study the mechanisms of stability of the flame.

The laser system used in this experiment consisted of a Quanta-Ray GCR 200 pulsed Nd:YAG laser, a Quanta-Ray MOPO-730 Optical Parametric Oscillator (OPO), and a Frequency Doubler Option (FDO). The GCR 200 pumped the OPO at a wavelength of 355 nm. Tuning of the laser beam wavelength was achieved through changes in the angle of the OPO crystals, Type I phase matched Beta Barium Borate (BBO). The gain of an OPO system is derived from the nonlinear interaction between an intense optical wave and crystal having a large nonlinear polarizability coefficient. The OPO used in this experiment was a coupled dual oscillator system where a high-energy power oscillator was injection seeded with the narrow output from a master oscillator. This enabled the coupled oscillator system to produce narrow bandwidth, high-energy, coherent radiation. The FDO extends the laser system wavelength output range into the ultraviolet for a total achievable wavelength range of 190 nm to 2000 nm.

For the laser induced fluorescence (LIF) measurements (Figure 3.2.6), the output of the OPO/FDO was focused into the flame by using a 1 m focal length fused silica bestform laser-focusing lens. The laser pulse power was monitored by placing a laser pulse energy meter at a position after the beam passed through the flame. This incident beam energy was used to normalize the LIF measurements for power variations. For the clear premixed flames of this study, laser attenuation through the flame was considered to be negligible.

The fluorescence signals were collected at a 90° angle of incidence to the input beam. The fluorescent signal was conditioned using emission wavelength specific optical filters before imaging to reduce stray light, background noise, and incident beam scattering.

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For the measurements of OH, a frequency doubled output of 285.265nm (Battles, et. al. 1994) of the OPO/FDO was used to induce fluorescence at a wavelength of ~315 nm (Hanson, 1986). These fluorescent signals were filtered through a narrowband filter (Melles Griot, Model 03 FIM 024). This filter has a center wavelength of 314.59 nm and a bandwidth (of 50% of the center wavelength) of 10 nm.

For the linear LIF (LLIF) measurements a Princeton Instruments Model ICCD-576-G/RB-E Intensified Charge Coupled Device (ICCD) was used to measure the LIF signal over the length of the traversing incident beam, thus giving a simultaneous profile of OH. The profile was developed by using a binning system consisting of summing the intensity of the pixels corresponding to the beam height (0.5mm) for each radial pixel using the WinSpec software. The signal was accumulated over 300 shots using a detection gate width of 10 ns, centered on the time of greatest fluorescence of the OH. A 10 ns gate width was chosen to reduce background noise.

The OH LIF detected fluorescence was quantified using the method of Laufer (1996). In this method, the number of detected photons was given by the relation:

$$n_{pe} = C_{exp} \times n_A \times C_{SV}$$
 3.3

where  $n_{pe}$  was number of detected photon,

 $C_{exp}$  was an experimental constant that describes the collection efficiency of the detection optics,

n<sub>A</sub> was the total number of OH molecules excited in the probe region, and

 $C_{SV}$  was the Stern-Volmer coefficient, which is a ratio of the molecules that transition due to a photon emission to the total number of excited molecules. The number of excited OH molecules was calculated using:

$$n_A = \frac{I_L}{hv_{ge}} n_{OH} \beta_{ge} \sigma_{ge} \Delta l$$
3.4

where  $I_L$  was the probe laser intensity,

h was the Plank's constant,

 $v_{ge}$  was the frequency of the probe laser,

 $\chi_{OH}$  was the mole fraction of OH in the probe region,

 $\beta_{ge}$  was the Boltzman fraction of excited OH molecules,

 $\sigma_{\rm ge}$  was the absorption cross section of OH, and

 $\Delta l$  was the length of the probe laser beam in the probe region.

Ideally, the number of photons emitted by OH would be equal to the number of excited OH molecules ( $n_A$ ) since each molecule will emit a photon as it transitions from the laser excited energy level to a lower energy ground state. However, emission of a photon is not the only mechanism of energy release for a molecule. Collisional quenching, dissociation of the molecule, ionization of the molecule and stimulated emission can be very important. However, for the low energy levels (~1mW maximum) of the exciting beam in this study dissociation, ionization, and stimulated emission losses were negligible (Hanson et al., 1990, Eckbreth, 1996). These assumptions allowed the Stern-Volmer coefficient to be written as:

$$C_{\rm SV} = \frac{A_{21}}{A_{21} + Q_{\rm C}}$$
 3.5

where A<sub>21</sub> was the Einstein spontaneous emission coefficient and

Q<sub>c</sub> was the quenching coefficient.

Combining the number of molecules excited (Formula 3.4) with the ratio of photons emitted for the total molecules excited (Formula 3.5) gives the total number of photons emitted from the test region. Unfortunately, not all emitted photons will be collected by the optics. The photons emitted radiate in all directions from the test region and the finite size of the collection optics can only collect a small percentage of these photons. Losses also occur through the transmission efficiency of the lenses, mirrors, and wavelength filters of the optics and through the detection efficiency of the photon detector. These losses were taken into account using the experimental constant  $C_{exp}$  given by:

$$C_{exp} = \left(\frac{\Omega}{4\pi}\eta_{T}\eta_{D}\right)$$
 3.6

where  $\Omega$  was the solid angle of collection of the optics,

 $\eta_{\rm T}$  was the combined transmission efficiency of the optics of the system (including any lenses, mirrors, and filters used), and

 $\eta_{\rm D}$  was the detection efficiency of the camera.

The collisional quenching component,  $Q_c$ , given in 3.6 is somewhat difficult to determine. Collisonal quenching is the reduction of a molecules energy level through the transfer of this energy by collisions with the other molecules of the gas mixture. Since there existed the potential for many species involved in collisional quenching for the measurements performed, each with their own quenching characteristics, the Garland and

Crosley (1986) expression for the total effect of collisional quenching was used. This was given as:

$$Q_{\rm C} = \sum_{\rm i} n_{\rm i} q_{\rm ix}$$
 3.7

where n<sub>i</sub> was the moles of collider species i and

q<sub>ix</sub> was the quenching rate of OH of the collider species.

Quenching rates have been studied extensively by a number of authors, particularly Paul et al (1995) and Tamura et al. (1998). Tamura et al. (1998) showed that the quenching rate for a collider species over a wide range of temperatures could be given as

$$q_{ix} = a_i \sigma_q T^{0.5}$$

and

$$\sigma_{q} = \sigma_{Q_{\infty}} \exp\left(\frac{\varepsilon}{kT}\right)$$
 3.9

where  $a_i$  and  $\sigma_{Q_n}$  are collider species experimental constants,

T was the gas temperature and

 $\varepsilon/k$  was an experimental constant for a given collider species (Table 3.3).

Planar Laser Induced Fluorescence (PLIF) images were collected in much the same way as LLIF data was collected. For PLIF, rather than a single beam passing through the flame as was used for LLIF, a cylindrical lens was used to create a laser sheet that passed through the flame. This created a 2-D field of radical fluorescence which was then imaged by a ICCD camera (Princeton Instruments Model ICCD-576-G/RB-E). Images were acquired and processed with a data acquisition computer using WinView software. Due to the limited field of view of the ICCD camera, the system was scanned

axially to create a composite image of the flame OH distribution. Due to variations in the intensity of the laser sheet, PLIF images are strictly qualitative.

#### **<u>3.3: Description of Test Matrix</u>**

In order to test the stability of the flames and to determine a percentage of hydrogen required to provide a wide range of testing conditions, the conditions given in Table 3.3a were used. The lift-off velocity and blow-off velocity of the three burners were determined for variations of hydrogen percentage in the propane/hydrogen mixture (10 to 100% by mass of hydrogen). This was done for a range of fuel mixture mass flow rates. Results of this testing will be presented in Section 4.1.

After the stability measurements were completed, a 40% by mass hydrogen in propane fuel mixture was used for all subsequent experiments. The rationale behind this choice will be given in Section 4.1.4. Table 3.3b gives the test matrix for the global characteristics of the burners. Measurements of flame length, CO, CO<sub>2</sub>, and NO emission index, radiative fraction, and radiative spectra were taken for jet exit velocities of 20 to 100 m/s and jet exit equivalence ratios of 0.55 to 4.0. These results are presented in Chapter 4.

Table 3.3c gives the test conditions for the flame structure measurements of this report. Profiles of CO, CO<sub>2</sub>, O<sub>2</sub> concentrations, temperature, axial velocity and RMS value of the turbulence component of axial velocity, and OH concentration were taken for a range of equivalence ratios and velocities of 20 m/s and 100 m/s. Schlieren and OH PLIF images were also taken. These results are presented in Chapter 5.

Experimental uncertainties are given in Table 3.4. The values shown are the 95% confidence intervals calculated through the Student "t' test.

Burner	Circular
Diameters	2.0 mm,
	3:1 Elliptical Aspect Ratio
	3.4 X 1.2 mm
	4:1 Elliptical Aspect Ratio
	4.0 X 1.0 mm.
Fuel	$H_2$ (95% and the rest inert)
Compositions	
	Propane (95.35% C <sub>3</sub> H <sub>8</sub> , 2.99%
	CH <sub>4</sub> , 0.92% C <sub>2</sub> H <sub>6</sub> , 0.74%
	$C_4H_8$ )
Jet Exit	20 m/s to 100 m/s
Velocity	
Jet Exit	1600-8000 (Depending on Fuel
Reynolds	Composition with Increased
Number	Equivalence Ratio Producing
	Higher Reynolds Numbers)
Ambient	295 K
Temperature	
Ambient	101 KPa
Pressure	

 Table 3.1: Nominal Experimental Conditions

Table 3.2: PDPA settings

Overall Settings		
Colliminating Lens	300 mm	
Transmission Lens	495 mm	
Receiver Aperture	100 µm	
Collection Angle	30° reflecting particles	
Photomultiplier Tube Voltage	600 V	
Velocity Spec	eific Settings	
Velocity	20 m/s	
Velocity Offset	5.00 m/s	
Velocity Range	-1.34 - 49.00 m/s	
Velocity Minimum	-5.00 m/s	
Velocity Maximum	80.00 m/s	
Measurement Range	-1.34 - 49.00 m/s	
Diameter Range	0.8 - 162.3 μm	
Diameter Maximum	10 µm	
Measurement Range	0.8 - 27.4 μm	

	$\sigma_{Q\infty}$	$\epsilon/k$	a
Collider	$(Å^2)$	(K)	$X 10^{-13} \text{ cm}^3 \text{s}^{-1}$
N <sub>2</sub>	0.4	624	4.47
O <sub>2</sub>	8	243	4.37
H <sub>2</sub> O	20	434	4.92
H <sub>2</sub>	4.5	224	10.88
CO <sub>2</sub>	11	488	4.16
СО	12	397	4.47
OH	20	384	4.99

Table 3.3:	<b>OH</b> Quenching	Constants
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Table 3.4a: Test Matrix (Stability Experiments)

	Fuel Mixture	
Burner Geometry	Hydrogen – Propane Mass %	Measured Parameters
Circular	100 % - 0 %	Equivalence Ratio/Fuel
3:1 Elliptic Aspect Ratio	50 % - 50 %	Jet Velocity at Lift off and
4:1 Elliptic Aspect Ratio	40 % - 60 %	Blow out
(All burners had equal	20 % - 80 %	
outlet areas corresponding	10 % - 90 %	
to an equivalent diameter		
of 2 mm)		

Table 3.4b: Test Matrix (Global Property Measurements)

	Burner Exit	Equivalence	
Burner Geometry	Velocity	Ratio	Measured Parameters
Circular	20 m/s	0.55	Flame Length, Emission
3:1 Elliptic Aspect Ratio	40 m/s	1.0	Index, Flame Radiation
4:1 Elliptic Aspect Ratio	60 m/s	2.0	
(All burners had equal	80 m/s	3.0	
outlet areas corresponding	100 m/s	4.0	
to an equivalent diameter			
of 2 mm)			

Burner Geometry	Burner Exit Velocity	Equivalence Ratio	Axial Location (% Flame Length)	Measured Parameters
Circular	20 m/s	0.55	12.5 %	OH Concentration,
3:1 Elliptic Aspect Ratio	100 m/s	1.0	25 %	Axial Velocity,
4:1 Elliptic Aspect Ratio		2.0	50 %	Schlieren Imaging,
(All burners had equal		4.0		Temperature
outlet areas corresponding				Profiles,
to an equivalent diameter of				Emission Profiles
2 mm)				

Table 3.4c: Test Matrix (Flame Structure Measurements)

 Table 3.5:
 Estimated Experimental Uncertainties (± Percentage of Mean)

Flame Length	10%
Temperature	10%
EI <sub>NO</sub>	9%
EI <sub>CO</sub>	8%
% CO	14%
% NO	9%
% O2	10%
OH	10%
<b>Radiative Fraction</b>	10%
Gas Velocity	6%


Figure 3.1.1: Schematic of Laboratory Combustion Chamber



Figure 3.1.2a: Fuel/Air Mixing Device Schematic



Figure 3.1.2b: Burner Holder Schematic



Figure 3.1.3a: Plan and Vertical Cross-Sectional Views of Burners



Circular Burner 5.1 Emptical Burner 4.1 Emptical Burner

Figure 3.1.3b: Photographic Images of Burners Viewed from the Top



Figure 3.1.4a: Cold Jet Velocity Profiles at 1 mm Above Circular Burner at a Bulk Jet Exit Velocity of 20 m/s



Figure 3.1.4b: Cold Jet Velocity Profiles at 1 mm Above 3:1 AR Elliptical Burner at a Bulk Jet Exit Velocity of 20 m/s



Figure 3.1.4c: Cold Jet Velocity Profile at 1 mm Above 4:1 AR Elliptical Burner at a Bulk Jet Exit Velocity of 20 m/s



Figure 3.2.1: Schematic of Schlieren Flow Visualization Setup



Figure 3.2.2: Schematic of Instrumentation for Rayleigh Scattering Measurements



Figure 3.2.3: PDPA Setup Schematic



Figure 3.2.4a: Apparatus for Measuring Global Emission of Flames



Figure 3.2.4b: Instrumentation for In-flame Species Concentration Measurements



Figure 3.2.4c: Gas Sampling Probe Design



Figure 3.2.5: Schematic of the Setup for Recording the Radiative Spectra



Figure 3.2.6: Experimental Setup for LIF/PLIF Measurements

# **CHAPTER 4: GLOBAL FLAME PROPERTIES**

## 4.1: Stability Results

The stability characteristics reported in this section deal with the parameters related to the overall behavior of the flame, specifically, the existence of the flame and the location at which the flame base exists. The flame conditions corresponding to stability are represented as follows: burner stabilized, lifted, partially lifted, blowout. A 'burner stabilized flame' is a flame where the flame base exists in close proximity to the burner rim. This is considered the most stable of the flame types. The base of a 'lifted flame' exists at a significant distance away from the burner. This flame is characterized by a cold jet of fuel or fuel/air mixture issuing from the burner which then propagates some distance (liftoff height) before reacting. A 'partially lifted flame' is when the flame is starting to exhibit signs of lifting off, but is still attached to the burner rim at some point. 'Blowout' represents the conditions where the flame ceases to exist.

**4.1.1 General Observations:** Stability measurements were taken by the following procedure. While maintaining a hydrogen/propane fuel mixture at a set hydrogen mass percentage and flow-rate, premix air was introduced slowly. The airflow rate at which liftoff and blowout occurred was recorded. This procedure was repeated for varying hydrogen/propane mixture fuel flow rates and hydrogen mass percentages in the fuel mixture. The reported Reynolds numbers were based on cold jet properties for the fuel/propane/air mixture used. Reported equivalence ratio was based on the amount of

air mixed with the fuel before it was delivered to the burner at the condition of liftoff or blowout.

Figures 4.1.1a through f and Figures 4.1.2a through f show the results of these experiments. To interpret these charts, the area above the data points represents the conditions that the flame blows out/partially lifts off. The area below the data points represents the flow conditions where the flame is stable and at least partially attached (Figs. 4.1.1a to f,) or is a lifted flame (Figs. 4.1.2a to f).

The first significant result was that for a given equivalence ratio, the velocity at which the flame blew out was only slightly higher (less than 5%) than that at which the flame lifts off the burner. The lifted flames were also very unstable at liftoff conditions often blowing out at slight disturbances of fuel jet inlet conditions or changes in ambient conditions. This instability accounts for the large gaps in data for some of the liftoff data in Figs. 4.1.2a to f. Therefore, for the premixed flames of this study, blowout essentially occurred immediately after the initiation of liftoff.

Lee and Chung (2001) found that for a propane/air premixed flame, if the fuel mass fraction is less than 0.6, the flame blows out without experiencing a lifted flame condition. This occurs because, upon liftoff, the non-combusting fuel jet that exists between the burner and the base of the lifted flame mixes with the surrounding air, effectively lowering the equivalence ratio of the premixed flame. The flame speed is lowered by this reduction of equivalence ratio and by the increase in dilution of the fuel mixture by ambient  $N_2$ , which will act to move the stabilization zone of the flame downstream. This increase in spacing between the burner and the flame allows even more air to mix with the fuel jet. This cycle continues until the flame reaches the lower

limit of flammability and extinguishes. The maximum fuel mass fraction in the present study was 0.14, well below the liftoff cut off of 0.6 fuel mass fraction for propane reported by Lee and Chung.

While hydrogen has a much lower lean flammability limit (at an equivalence ratio of 0.14 compared to 0.51 for propane), the enhancement of stability provided by the hydrogen addition to the fuel should not affect the behavior of blowing out immediately after liftoff significantly since the feed back loop of decreasing equivalence ratio mentioned above would still be in effect.

The figures show that an increase in the hydrogen percentage of the fuel mixture increased the maximum jet exit velocity attainable for a given equivalence ratio of the jet for both partial liftoff and blowout. Hydrogen is a fast reacting species (i.e., high flame speed), so it increases the range of velocities over which the flame is stable primarily through an increase in flame velocity allowing the flame to establish on the lip of the burner easier thus resisting liftoff.

At conditions immediately prior to blowout, it was observed that, for the circular burner, the flame would erratically partially lift off of the edge of the burner exit. While the flame was partially lifted off, the flame would produce a large high frequency hissing sound indicative of high turbulence levels. As the jet exit velocity was increased, the length of time of partial liftoff would increase, and the partial liftoffs would become more frequent in occurrence. Blowout would occur by having a partial liftoff zone propagate completely around the burner exit. The flame would then lift off and blow out. The 3:1 aspect ratio (AR) elliptical burner flame behaved similarly to the circular burner flame in the blowout behavior described above. The 4:1 AR elliptical burner flame also exhibited partial liftoffs, but these liftoffs tended to occur at the ends of the major axis. At conditions immediately before liftoff/blowout, the 4:1 AR elliptical burner flame would lift off at both ends of the major axis but would maintain attachment to the burner along the minor axis.

For the burners of this study, the stability curves consisted of, in general, three regions. The first, which occurred at lean to slightly rich equivalence ratios (a range of 0.3 to 1.4), was a region with a slow, linear increase in maximum obtainable jet velocity before blowout with increase in jet exit equivalence ratio. The second consisted of, at slightly to moderately rich equivalence ratios (equivalence ratios of 1.4 to 2.0), a region where the maximum obtainable burner exit velocity before blowout showed a stronger dependence on equivalence ratio with small increases in equivalence ratio allowing much greater burner exit velocities. The third region was where the maximum obtainable jet velocity before blowout again became a weaker function of the equivalence ratio and increased slowly with it. The third region occurred at moderate to very rich equivalence ratios (equivalence ratios of 2.0 to the maximum equivalence ratio tested).

The beginning of a transition from a laminar to a turbulent flame was likely the reason for the first inflection in the stability charts. In general, the first inflection appeared in the vicinity of Reynolds number of 5000 (Figs. 4.1.1d through f) which was where the transition to turbulence initiated (to be further discussed in Section 4.1.5). The second inflection point was likely the point at which the flame became fully turbulent. The increased slope of velocity between inflections was a result of the combination of the change in laminar flame speed for varying equivalence ratio and the large increase of flame speed provided by small-scale turbulence as described by Damkohler (Kanury

(1975)). The slope decreased in region three due to the smaller increase in flame velocity caused by large scale turbulence.

**4.1.2 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** From Fig. 4.1.1a, it can be seen that the circular burner had a narrower range of equivalence ratios where the maximum attainable burner exit velocity before blowout increased dramatically with a small increase in equivalence ratio (Region 2 as described previously). Up to a certain hydrogen content, with increasing percentages of hydrogen in the fuel mixture, the slope of the curve of maximum attainable jet exit velocity increased with increasing equivalence ratio and then the trend reverses.

For the circular burner, for the 100%  $H_2$  flame, the region of greatly increasing maximum attainable velocity with increasing equivalence ratio was for a range of equivalence ratios of 0.4 to 1.2 with a slope of 140 m/s per unit increase in equivalence ratio, for the 50% by mass of hydrogen in propane mixture this range of equivalence ratios was from 0.9 to 1.3 with a slope of 180 m/s per unit increase in equivalence ratio, and for the 40% hydrogen by mass mixture it was from equivalence ratios of 0.8 to 1.4 with a slope of 101 m/s per unit increase in equivalence ratio.

In comparison, with the 3:1 AR elliptical burner (Fig. 4.1.1b), the extent of the increase in maximum attainable jet exit velocity with increase in equivalence ratio was not as strong. For the 100% hydrogen fuel, the large increase in maximum attainable jet velocity occurred in the range of equivalence ratio of 0.4 to 1.4 with a slope of 100 m/s per unit increase in equivalence ratio. For a 50% hydrogen by mass mixture the slope from an equivalence ratio of 1.0 to 1.8 was 61 m/s per unit increase in equivalence ratio.

The 40% by mass mixture had a range of increased slope of maximum obtainable jet exit velocity of equivalence ratios of 1.4 to 2.0 with a slope of 52 m/s per unit increase in equivalence ratio.

From a turbulence stability chart (Fig. 4.1.3) that will be discussed later in Section 4.1.5, the 3:1 AR elliptical burner tended to transition to a turbulent flame much earlier than the circular burner; this transition occurred at a Reynolds number of about 4500 for the 3:1 AR burner and a Reynolds number of about 6500 for the circular burner. From Figs. 4.1.1d and e, these transition Reynolds numbers correspond to where the slope of the stability curves changed for the circular and 3:1 AR elliptical burners. The increase in turbulence had the effect of increasing the flame speed allowing the flame to stay attached to the burner for a greater jet exit velocity, thus, the increase in slope.

However, for the 3:1 AR elliptical burner, the increased mixing inherent to elliptical burners will tend to reduce the local equivalence ratio at the burner exit (due to mixing with the surrounding air). This reduction in equivalence ratio (and thus potential reduction in flame speed) may overwhelm the increase of turbulent flame speed, thus giving the lower maximum jet exit velocity before blowout for the 3:1 AR elliptical burner compared to the circular burner. Also, the extent of the region of large increase of flame speed due to small-scale turbulence described by Damkohler is a strong function of the burner geometry. Given that the 3:1 AR elliptical burner had an increased turbulence production, the transition from small scale to large-scale turbulence will occur faster. This smaller transition was why the second region of increased velocity slope does not strongly appear in the 3:1 AR elliptical burner stability curves compared to what was seen for the circular burner.

It was apparent that the use of the 3:1 AR elliptical burner at Reynolds numbers greater than 5000 caused a reduction in blowout stability (i.e. the maximum premixed gas jet velocity attainable was lower for a given equivalence ratio) compared to the circular burner. This was in agreement with the results for elliptical diffusion flames found by Gollahalli et al. (1992).

The reduction in blowout stability was due to the decreasing of the local equivalence ratio in the flame anchoring zone for a given Reynolds number. At Reynolds numbers lower than 5000, the stability of the 3:1 AR elliptical and circular burners was similar. This was due to both flames being laminar thus the enhanced turbulence generation of the elliptical burner was not present to affect the fuel jet.

**4.1.3 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:** For a given Reynolds number, the 4:1 AR elliptical burner (Fig. 4.1.1c) had a greater maximum obtainable jet exit velocity than the 3:1 AR elliptical burner, for all cases except the 10% hydrogen by mass hydrogen/propane mixture. The 4:1 AR elliptical burner could attain a higher maximum jet exit velocity for a given equivalence ratio because a bifurcation of the 4:1 AR elliptical burner flame (which will be discussed later) introduced a large rate of velocity decay. The 4:1 AR elliptical burner also tended to transition to turbulence later than the 3:1 AR elliptical burner (Fig. 4.1.3). This lowering of velocity and delay of turbulence initiation apparently counteracted the destabilization effect of the ellipticity of the 4:1 AR elliptical burner.

Similar to the circular burner, the 4:1 AR elliptical burner also tended to have regions where the maximum obtainable jet exit velocity was particularly strong function

of the equivalence ratio. For the 100% hydrogen flame, this was a range of equivalence ratios of 0.5 to 1.0 with a slope of 220 m/s per unit increase in equivalence ratio, for the 50% by mass hydrogen flame, the range was of equivalence ratios of 1.0 to 1.4 with a slope of 170 m/s per unit increase in equivalence ratio, and for the 40% by mass hydrogen mixture the range was for the range of equivalence ratio of 1.0 to 1.7 with a slope of 90 m/s per unit increase in equivalence ratio. It would appear that, unlike the 3:1 AR elliptical burner, the 4:1 AR elliptical burner still maintained a significant range of velocities where small scale turbulence dominates, thus the presence of the regions of high velocity slope.

**4.1.4 Determination of Hydrogen Percentage for Flame Structure Studies:** From the above described stability results, a hydrogen mass percentage of 40% was chosen for future experiments to allow a broad range of equivalence ratios and bulk gas velocities for stable flames. This hydrogen mass percentage was chosen because it was desired to have a flame that was stable over a wide range of conditions but still maintained a significant hydrocarbon percentage for facilitating studies of the relative effects of premixing and ellipticity on CO and  $CO_2$  emissions. All subsequent measurement and analysis were performed using a hydrogen/propane mixture with a 40% by mass hydrogen/propane mixture for varying equivalence ratio and bulk jet exit velocity are given in Table 4.1.1.

**4.1.5 Laminar-Turbulent Transition:** The point where the flame began the transition between a laminar and turbulent flame was determined in a similar manner as the flame stability curves. A 40% hydrogen to propane by mass mixture was sent to the burner and the premix air was gradually increased (simultaneously lowering the equivalence ratio and increasing the Reynolds number). Turbulence initiation was determined to occur when the flame began to emit a medium pitched hiss/roaring sound. This was accompanied by the development of a region near the top of the flame of somewhat higher visual intensity. This higher visual intensity indicated a faster reaction speed indicative of the enhanced mixing provided by turbulence. These results are presented in Fig. 4.1.3. Conditions located above the data points were regions of transitional turbulence; those below the data points were laminar flame conditions.

The 3:1 AR elliptical burner initiated transition to a turbulent flame from Reynolds numbers of 4000 to 4500, the 4:1 AR elliptical burner initiated transition from Reynolds numbers of 4500 to 5000, and the circular burner initiated transition between Reynolds numbers of 5000 to 6500. For a given equivalence ratio, the circular flame maintained laminar conditions for higher Reynolds numbers than the 3:1 AR and 4:1 AR elliptical burners. The elliptical burners tended to transition to turbulent conditions earlier due to enhanced vortex generation (Hussain and Husain (1989), Kamal (1995)). This increased turbulence for the elliptical burners was confirmed from PDPA velocity measurements given in Section 5.1.1.

Comparing elliptical burners, the 4:1 AR elliptical burner could attain a higher Reynolds number before transitioning than the 3:1 AR elliptical burner. The 4:1 AR

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elliptical burner bifurcated creating a large velocity decay rate. This velocity decay suppressed the initiation of turbulence by lowering the local Reynolds number of the jet.

The elliptical burners had a mild increase in the transition Reynolds number with increasing equivalence ratio while the circular burner showed a stronger increase in transition Reynolds number with increase in equivalence ratio. The increase of transition Reynolds number with increasing equivalence ratio was due to an increase in temperature, with subsequent increase in gas viscosity. Since a higher velocity will be required to achieve a similar 'flame' Reynolds number, this manifests as an increase in the cold jet Reynolds numbers.

The reduced slope of the elliptical burners, compared to the circular burner, indicated that the elliptical burners, in addition to transitioning earlier than the circular burner, had transition Reynolds numbers that were more a function of burner geometry than the properties of the flame jet. This is reasonable due to the enhanced turbulence generating properties of the elliptical burners overwhelming the natural turbulence development of the jet.

## 4.2: Flame Appearance

**4.2.1 General Observations:** The circular, 3:1 AR elliptical, and 4:1 AR elliptical burners (Figs. 4.2.1 a, b, c, d, and e and Figs. 4.2.2 a, b, c, d, and e) showed general combustion aspects typical to premixed laminar flames in other studies (Smooke, et. al., (1988), Turns (1996), and Xiao et al. (2000)). For equivalence ratios of 3.0 or less, two flame regions were visible with all three burners of this study. The more striking of the two regions was a high intensity blue region located near the burner. A second faint blue region of much lower luminous intensity surrounded the bright inner flame. The bright blue region was the premixed combustion/fast reaction zone of the flame. In this zone, the premixed air and fuel reacted, and fast reaction mechanisms (such as hydrogen oxidation) occurred. The surrounding flame zone was where any remaining unburned components mix with the surrounding air (as a diffusion flame), and where slower combustion reactions (such as the CO to  $CO_2$  reaction) occurred.

In general, for the 3:1 AR and circular flames, the bright blue (premixed) region had a width slightly greater than the apparent diameter of the burner outlet on both the major and minor axis. Just above the outlet, the flame narrowed with increase in axial length. The region of the premixed flame at its tip (the point furthest from the burner) had a rounded shape due to the proximity of the bounding flame fronts. This rounding of the 'point' of the bright blue flame was also reported by Echekki and Mungal (1990). This proximity of the bounding flame fronts with the low volume rate of incoming reactants allowed increased preheating. This preheating increased the flame speed (to as much as a factor of 6.25 (Echekki and Mungal (1990)), through increases in the reaction rate, which allowed the flame to stabilize at a higher velocity creating the rounding effect. The 4:1 AR elliptical burner flame had the visual appearance of a single reacting jet close to the burner, but the flame rapidly split into two reacting jets. A blue-green 'yoke' of slightly lower intensity bridged the two premixed flame jets near the burner. This splitting occurred because of a bifurcation of the 4:1 AR elliptical jet flow. The bifurcation resulted in increased mixing with the surrounding air and had a great effect on the flame length and emissions of the flame, as will be shown. A close examination of the 3:1 AR elliptical burner at an equivalence ratio of 0.55 also suggested a small amount of bifurcation for the premixed region. In the region downstream of the complete bifurcation of the 4:1 AR elliptical burner's premixed flame, the sub flames had an overall appearance similar to the circular and 3:1 AR elliptical flames.

**4.2.2 Effect of Level of Premixing:** The visible intensity of the premixed flame was at a maximum at an equivalence ratio of 1.0. For an equivalence ratio of 0.55, the premixed flame had a paler blue hue. As the burner exit equivalence ratio increased from stoichiometric, the premixed region became less visually intense and increased in length. The diffusion flame region also increased in length. For the circular and 3:1 AR elliptical burners at equivalence ratios of 4.0 or greater, the inner premixed region was no longer visible, however, there was a slight inner blue region in the 4.0 equivalence ratio 4:1 AR elliptical flame. It was likely that enhanced mixing of the 4:1 AR elliptical burner created a lower local equivalence ratio thus intensifying the premixed region relative to the 3:1 AR elliptical burner. Alternately, the 4:1 AR elliptical burner had greater combustion intensity due to reduction of flame length/reduction in jet velocity which increased the radiative emissions.

It is noteworthy that the flames with equivalence ratios of 0.55 and 1.0 for the three burners still maintained the outer diffusion region (although it was greatly reduced compared to the fuel rich cases) when, by definition, sufficient oxidant was present for complete combustion in the premix flame zone. The residence time in the premixed region was too small to allow complete combustion, so the diffusion region existed due to the slower reactions taking place after the premix combustion. This two stage flame behavior was common to both the circular, 3:1 AR elliptical, and 4:1 AR elliptical burners.

**4.2.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** Overall, the flame structure of the 3:1 AR elliptical and circular burner was similar (Figs. 4.2.1a, b, and c and Figs. 4.2.2a, b, and c). Close to the burner outlet, the 3:1 AR elliptical burner viewed perpendicular to the major axis showed a broadening of the premixed flame region and an apparent narrowing of the surrounding diffusion flame zone compared to the circular burner. Broadening of the premixed flame region was due to a wider fuel jet (aspect ratio effect), while the narrowing of the outer flame zone was due to the enhanced mixing of the elliptical burner with the surrounding air. Since, for rich premix conditions, the outer flame was essentially a diffusion flame, increased mixing allowed faster combustion which led to flame narrowing.

The phenomenon of axis switching seen in both cold jet (Ho and Gutmark (1987) report three axis switchings in the range of 40 diameters from the nozzle and Khanna (1990) reports axis switching at 10, 20, and 26 diameters from the nozzle) and flame conditions (Gollahalli et al. (1992)) observe axis switching at 20, 30, and 40 diameters

for a diffusion flame) was suggested by the 3:1 AR elliptical flame images (Fig. 4.2.3) but was partially obscured by the narrowing of the premixed region of the flame.

For the 3:1 AR elliptical flames of this study, an axis switching of the visual width of the premixed flame appeared to occur at an x/d of 5 (at an axial distance of 1 cm) for the premixed flame cone. Above this location, the minor axis premixed region was much wider visually than in the major axis plane, particularly for Reynolds numbers of 5700 and greater. The outer diffusion flame did not appear to have an axis switching: the minor axis visible flame width was always wider than the major axis visible flame width.

There are several reasons for the discrepancy between axis switching locations between the flame conditions of Gollahalli et al (1992) and the conditions of the current study. The natural narrowing of the inner cone of the flame obscured any other axis switchings and could contribute to the axis switching appearing so close to the burner compared to the diffusion flame results. Also, Gollahalli et al. (1992) worked with a turbulent diffusion flame in their studies and defined axis switching based on the velocity half width of the jets. The current study estimates axis switching from visual flame measurements on a laminar flame.

**4.2.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:** There were significant differences in the flame structure between the 3:1 AR elliptic and 4:1 AR elliptic burners (Figs. 4.2.1b, c, d, and e and Figs. 4.2.2b, c, d, and e). In the 4:1 AR elliptic burner, both the inner premixed region and the outer diffusion flame split. Visually, this appeared to take the structure of two fuel jets emitting from the burner at an angle of 10 degrees from the burner centerline, with a somewhat lower intensity blue region yoked between the two jets. The angle between the diverging jets was constant for all equivalence ratios and velocities. In addition, the 4:1 AR elliptical flame tended to be much shorter in length and broader in width. The flame was shorter due to the enhanced mixing due to bifurcation, and with the increased flame circumference, due to the creation of two jets, a shorter height is necessary for a given volume of reaction.

The premix region of the 4:1 AR elliptical burner sub flames appeared elliptical in shape and were oriented parallel to the minor axis (i.e. rotated 90 degrees from the major axis). This ellipticity can be seen in the comparison of the major and minor axis images for the 4:1 AR elliptical flames. In Fig. 4.2.1d, the width of the premix flame downstream of the flame yoke was narrow while it was wider in Fig. 4.2.1e. The outer diffusion flame did not exhibit this ellipticity.

## **4.3:** Flame Length Measurements

**4.3.1 General Observations:** For a constant bulk jet velocity of 20 m/s, the overall (diffusion region) flame length was measured for a range of equivalence ratios from 0.55 to 4.0 (Fig. 4.3.1a), while the premixed flame length was measured from equivalence ratios of 0.55 to 3.0 (Fig 4.3.1b). Measurements of flame length are also presented for varying jet exit Reynolds numbers with constant equivalence ratios of 2.0 and 4.0 in Figs. 4.3.2a and b and Fig. 4.3.3. The equivalence ratio of 4.0 results are presented for a range from 20 to 100 m/s bulk jet velocity, corresponding to Reynolds numbers of 1600 to 8000, while the equivalence ratio fixed at 2.0 experiments range from 20 to 80 m/s bulk jet velocity (Reynolds number of 1900 to 7500). The reduced velocity range for the equivalence ratio of 2.0 results was due to flame extinction occurring at a 100 m/s bulk jet velocity.

**4.3.2 Effect of Level of Premixing:** For a bulk jet velocity of 20 m/s, in general, an increase in equivalence ratio caused an increase in flame length for both the overall and premixed flame lengths (Fig. 4.3.1a and b). This was as expected since the reduced amount of premixing of air (with the proportional increase of fuel in the jet) creates a longer required reaction time by increasing the amount of unburned products remaining after premixed combustion (Rokke et al. (1994), Kim et al. (1995), Lee et al. (1997) and Xiao et al. (2000)).

For the overall flame length, the region of equivalence ratios of 0.55 to 2.0 tended to have a higher sensitivity to equivalence ratio changes than in the range of equivalence ratios of 2.0 to 4.0. This higher slope for the lean to moderately rich

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equivalence ratios was caused by the rapid increase in incomplete reaction products leaving the premixed flame zone with increasing equivalence ratio.

For equivalence ratios greater than 2.0, the flame began to approach diffusion flame conditions. In these cases, much of the fuel left the premixed flame zone without completely burning, thus flame length became increasingly mixing dominated. Even though, for a constant burner exit velocity, overall flame length is expected to be constant for a diffusion flame, in the present case it increased due to higher rate of fuel input with increasing equivalence ratio. The premixed flame length was less dependent on equivalence ratio at lower equivalence ratios but more dependent for rich mixtures.

The length of the premixed region is a function of the local flow velocity and the speed of propagation of the flame (Turns (1996)). The premixed flame front is established where these conditions are balanced. Changes of the fuel/air equivalence ratio from unity tend to lower the flame speed. For equivalence ratios greater than 1.0, the availability of oxygen became a limiting factor causing the flame speed and temperature to be reduced. This tended to move the flame front further downstream in the flame. For fuel lean flames, the total amount of oxidant was of lesser importance (since all oxygen needed for combustion is present already), so the effect of equivalence ratio on flame length was reduced.

There was a significant difference between the flame length behavior of varying bulk jet velocity with fixed equivalence ratio of 2.0 (Fig. 4.3.2a and b) and fixed equivalence ratio of 4.0 (Fig. 4.3.3). For an equivalence ratio of 4.0, the circular and 3:1 AR elliptical burners exhibited a sharp increase in the overall flame height with increase in Reynolds number in the 2000 to 3000 range. For Reynolds numbers greater than 3000,

the overall flame length decreased. This was due to a transition from a laminar to turbulent flame.

For the fixed equivalence ratio of 2.0 case, there was a small increase in overall flame length for the range of Reynolds numbers of 2000 to 5000. For Reynolds numbers greater than 5000, the 3:1 AR elliptical burner flame decreased in length by 20% while the circular burner flame length increased in length by 37%. Again, the 3:1 AR elliptical burner tended to transition to turbulent flow earlier than circular, as shown in Fig 4.1.3, causing the reduction in flame length. The circular flame was still in a laminar regime (or just beginning to transition to turbulence for the Reynolds number of 7500 flame) which tended to produce a longer flame.

For both the equivalence ratios of 2.0 and 4.0, the 4:1 AR elliptical burner flame length was constant, thus the 4:1 AR elliptical burner flame length was not a strong function of Reynolds number (thus turbulence level) and was determined primarily by geometry and equivalence ratio effects.

**4.3.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** For the 20 m/s fixed velocity case with varying equivalence ratio, both the overall and premixed flame lengths were very similar for the circular and the 3:1 AR elliptical burners (Fig 4.3.1a and b). This indicates that elliptical effects on flame length were minor for lower aspect ratio elliptical burners corresponding to a jet exit velocity of 20 m/s (Reynolds number of 1900). This absence of elliptical effects on flame lengths at lower Reynolds numbers will be mirrored in the varying Reynolds number comparisons below.

For a constant equivalence ratio of 2.0 (Fig. 4.3.2a and b), the overall flame length of the circular burner was greater than the 3:1 AR elliptical burner for Reynolds numbers greater than 2000. Below a Reynolds number of 2000, the circular and 3:1 AR elliptical burner flames were laminar, thus their flame lengths were similar. From Fig. 4.1.3, the 3:1 AR elliptical burner flame transitioned to turbulence earlier than the circular flame, so for Reynolds numbers greater than 2000 the effects of the turbulence shortening the flame for the 3:1 AR elliptical burner became apparent. The flame lengths for the circular and 3:1 AR elliptical burner increased slowly in the range of Reynolds numbers of 4000 to 6000 with circular burner showing a higher increase. The difference in flame length became most pronounced at a Reynolds number of 7500 where the 3:1 AR elliptic burner flame length decreased slightly and the circular burner flame length increased.

For the premixed flame of equivalence ratio of 2.0, the circular and 3:1 AR elliptical burners produced very similar lengths in the range of Reynolds numbers of 2000 to 4000. At a Reynolds number of 5600, the circular burner developed a significant increase in premixed flame height compared to the more moderate gain exhibited by the 3:1 AR elliptical burner. At a Reynolds number of 7500, the circular premixed flame increased in length by 71%, while the 3:1 AR elliptical burner increased 41%. This continued increase in the premixed flame length despite the decrease in the overall length indicates that the flame was in a transitional turbulent regime (with its attendant shortening of overall flame lengths) occurring above the premixed region. This can be seen in Figs. 4.2.2b and c for the Reynolds number of 7500 flame.

For a constant equivalence ratio of 4.0, the circular and 3:1 AR elliptical burners showed similar trends. Both showed a similar and increasing overall flame lengths with increase of Reynolds number of 1600 to 3000 and a decrease in overall flame length for increase in Reynolds number from 3000 to 8000. The 3:1 AR elliptical burner flame length decreased faster with increased Reynolds number than the circular burner. This was due to the earlier transition to a turbulent regime with the 3:1 AR elliptical burner. For Reynolds numbers greater than 3000, the 3:1 AR elliptical burner had a shorter flame length than the circular burner.

**4.3.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:** For a constant 20 m/s bulk velocity with varying equivalence ratio (Fig 4.3.1a), the 4:1 AR elliptical burner produced flames of half the overall length as that of the 3:1 AR elliptical burner. This shortening of the flame was due to three potential reasons. The first was the enhanced mixing associated with elliptical jets. Potentially better mixing by the 4:1 AR elliptical burner leads to more rapid burning and, thus, produces a shorter flame. Secondly, the two jets of the bifurcated flame had a greater reaction surface area which allowed faster combustion of the fuel. Finally, a reduced jet velocity due to the increased velocity decay rate of the 4:1 AR elliptical burner allows a greater residence time for the flame.

An examination of the height of the premixed region (Fig. 4.3.1b) reveals similar conclusions as that for the overall flame length. In general, the 3:1 AR elliptical burner produced longer premixed burning regions than the 4:1 AR elliptical burner, for any given equivalence ratio. This was likely due to the 4:1 AR elliptical burner having a

greater velocity decay rate than the circular burner, thus allowing the establishment of the laminar premixed flame front at a lower height. At equivalence ratios of less than or equal to 1.0, the difference between the bright blue region lengths was small. This was due to the enhanced mixing of the 4:1 AR elliptical burner causing the fuel air mixture to become sufficiently lean to lower the laminar flame speed, thus delaying the development of the flame front.

As the equivalence ratio was held constant at 2.0 and the velocity was varied (Fig. 4.3.2a and b), the following trends were apparent. The overall flame length of the 3:1 AR elliptical and the 4:1 AR elliptical burners were only weakly dependent on Reynolds number with the flame length of the 3:1 AR elliptical burner being twice the length of the 4:1 AR elliptical burner. The premix flame length increased with increasing Reynolds number for the 3:1 AR elliptical burner. The 4:1 AR elliptical burner had a slight increase in premixed flame length with increase in Reynolds number.

At a premixed equivalence ratio of 4.0 with varying velocity (Figure 4.3.3), the 3:1 AR elliptical burner flame length showed a dependence on the bulk jet velocity while the flame length of the 4:1 AR elliptical burner was constant. At these rich flame conditions, flame length is a strong function of the mixing rate with the surrounding air. Until a Reynolds number of approximately 3100, the 3:1 AR elliptical burner flame was still entirely laminar, with a consequent low mixing rate. At Reynolds numbers greater than 3100, the 3:1 AR elliptical burner flame began to transition to a turbulent regime with enhanced mixing. This transition created the reduction in flame length apparent in the figure. The 4:1 AR elliptical burner had enhanced mixing independent of turbulence level due to fluid dynamic effects and behaved like a fully-turbulent momentum

dominated flame. Thus, the flames remained short for the 4:1 AR elliptical burner regardless of the turbulence level.

#### 4.4: Emission Index Results

**4.4.1 General Observations:** Flames of this study were premixed, so they were characterized by very low CO emissions. For constant velocity with varying equivalence ratio (Figs. 4.4.1a, b, and c), the circular and 3:1 AR elliptical burners produced similar CO and NO emissions across the range of equivalence ratios. The 4:1 AR elliptical burner produced higher CO and lower NO than the other two burners.

For the laminar flame, the circular burner produced CO emissions in a range of 0.5  $g_{co}/kg_{fuel}$  to 1.25  $g_{co}/kg_{fuel}$  and NO emission in the range of 1.0  $g_{NO}/kg_{fuel}$  to 4.0  $g_{NO}/kg_{fuel}$ . This was somewhat higher than the results reported by Kim et al. (1995) where, for a similar variation in equivalence ratio, a laminar premixed, co-flow C<sub>2</sub>H<sub>6</sub> flame produced a range of CO production of 0.32  $g_{CO}/kg_{fuel}$  to 0.72  $g_{CO}/kg_{fuel}$  and a range of NO of 1.2  $g_{NO}/kg_{fuel}$  to 1.48  $g_{NO}/kg_{fuel}$ . The current studies results were much greater than reported by Gore and Zhan (1996) in their study of an enclosed laminar CH<sub>4</sub> flame. Their burner produced a range of 0.041 to 0.06  $g_{CO}/kg_{fuel}$  and 0.84 to 1.0  $g_{NO}/kg_{fuel}$ .

From a study of turbulent premixed flames by Lyle et al. (1998), it was observed that confined flames tended to produce much less CO for a given burner equivalence ratio than unconfined flames. This tendency will likely be true for a laminar flame also. Gore and Zhan (1996) used a confined flame, so CO would be expected to be lower. For the study by Kim, there was a combination of the effects of co-flow and of the use of  $C_2H_6$  as the fuel (a lower hydrocarbon than  $C_3H_8$ ), which should both reduce CO production. However the addition of hydrogen to the current fuel should reduce the increase due to the use of  $C_3H_8$  (by changing the effective C/H ratio of the fuel. NO production is a strong function of flame temp, and the  $H_2/C_3H_8$  mixture used in this study has an adiabatic flame temperature much greater than the fuels of the previous studies (CH<sub>4</sub> is 2226K, C<sub>2</sub>H<sub>6</sub> is 2259K, and the current mixture is 2334K), so it should have higher NO emissions. For equivalence ratios greater than 2.0 the NO increased with increasing equivalence ratio for the previous studies and the current flames. However Kim and Gore showed a peak NO production at an equivalence ratio around 1.5. This peak was attributed to formation of NO due to the prompt mechanism. Since volumetrically, the C<sub>3</sub>H<sub>8</sub> component was small for the mixture of this study, prompt NO production (which has CH as a key radical) will be very small, so the peak was not seen with the current fuel mixture.

With varying burner exit Reynolds number at a constant equivalence ratio of 2.0, the elliptical burners produced greater CO for Reynolds numbers greater than 4000 and reduced NO at Reynolds number of 7600 compared to the circular burner. At a fixed equivalence ratio of 4.0 with varying burner exit Reynolds number (Figs. 4.4.2a and b, and Figs. 4.4.3a and b), the elliptical burners tended to produce greater CO and reduced NO compared to the circular burner.

For Reynolds numbers greater than 4000 the results are in contrast to turbulent diffusion flame results (Gollahalli et al. (1992), Kamal, (1995)), which showed that elliptical diffusion flames tended to produce lower CO than circular diffusion flames while producing similar NO. In diffusion flames, the enhanced mixing of the fuel jet with surrounding air provided by the elliptical burners increases the combustion efficiency and temperature of the flame, with a corresponding decrease in CO. In

premixed flames, since the fuel and air are already combined, mixing of the fuel jet with surrounding air is of less importance for oxidation.

For the higher Reynolds number flames of this study, the reduction of the elliptical burner flame length takes an important role in the characteristics of the flame. A reduced flame length implies, for a given bulk gas jet velocity, a reduced residence time within the reaction zone of the flame. This reduced residence time results in a higher CO and lower NO production due to the relatively long reaction times required for CO to  $CO_2$  and N to NO reaction. Also, the enhanced mixing may cause a tendency of a reduction of the flame gas temperature by mixing with outside air sufficient to freeze the flame reactions, extinguishing the flame before complete combustion has occurred. While the temperature at the core of the flame is unlikely to be dropped significantly by this mixing, the quenching effect is greater at the edge of the flame as will be seen in Chapter 5.

For the turbulent flame, at an equivalence ratio of 4.0 the circular burner produced a EICO of 3.0  $g_{CO}/kg_{fuel}$  and a EINO of 2.6  $g_{NO}/kg_{fuel}$  at a Reynolds number of 8000 which was in reasonable agreement with Turns et al. (1993), and Lyle et al. (1998). Turns reported that their turbulent premixed C<sub>3</sub>H<sub>8</sub> flame produced 2.6  $g_{NO}/kg_{fuel}$  at an equivalence ratio of 5.0 (the lowest equivalence ratio tested for propane by Turns) and 2.0  $g_{NO}/kg_{fuel}$  for a CH<sub>4</sub> flame at an equivalence ratio of 4.0. CH<sub>4</sub> flames tended to produce lower NO than the C<sub>3</sub>H<sub>8</sub> flame for a given equivalence ratio in their study. Lyle reported a NO production of 2.2  $g_{NO}/kg_{fuel}$  for an unconfined with co-flow turbulent CH<sub>4</sub>/air premixed flame of equivalence ratio of 4.0. For CO production, the turbulent flames at equivalence ratio of 4.0 of the current study produce an order of magnitude greater EICO ( $3.0 \text{ g}_{\text{CO}}/\text{kg}_{\text{fuel}}$ ) than the flames of Lyle, et. al ( $0.3 \text{ g}_{\text{CO}}/\text{kg}_{\text{fuel}}$ ). Again, the use of CH<sub>4</sub> as the fuel and co-flow by Lyle will be, at least partially, responsible for this discrepancy.

**4.4.2 Effect of Level of Premixing:** As shown in Figures 4.4.1a and b, an increase in the equivalence ratio caused CO emission indices to decrease, and NO emission indices to increase for all three burners. These effects were greatest in the region of equivalence ratios of 0.55 to 1.0 for CO and for the region of equivalence ratio of 0.55 to 2 for NO. These results are contrary to what is expected and what was seen in Kim et al (1995) and Gore and Zhan (1996). It would be thought that a decrease in available oxygen (with the higher equivalence ratios) would reduce the degree of complete combustion and, thus, increase CO levels. Also for a lower degree of complete combustion, it would be expected to have lower flame temperatures and thus lower NO production.

There are two probable reasons why the burners of this study gave unexpected carbon monoxide emission index results. First, with enhanced mixing, there is the potential, at lower equivalence ratios, that sufficient air will be mixed with the combusting jet that the local equivalence ratio will be lowered to beyond the lean flammability limits (Guj, et. al. (2001), Schefer (2003)) extinguishing the flame. For a premixed, methane fueled gas turbine, Schefer reported that the CO emission begins to rapidly increase for equivalence ratios less than 0.44, an equivalence ratio close to that used for the premixed flames of this study. Secondly, the local temperature could be reduced to a point where CO reaction rates will become very small (Correa (1992)). The

reduction in temperature to below CO reaction rate limit is made easier by the fact that the flame temperature of lean mixtures is reduced compared to that at stoichiometric conditions, thus less mixing is necessary to create a drop in temperature. This is particularly the case for the small flames (2 mm equivalent outlet diameter) of this study. This can be seen by the observation that the 4:1 AR elliptical flame with its bifurcation enhanced mixing produced higher CO.

The increase of NO with increase in equivalence ratio exhibited by the current study was also observed by Driscoll et al. (1992) in their study of partially premixed hydrogen air flames of Reynolds number of 5000. The explanation for this increase of NO is that, while the combustion will be more efficient with higher premixing, the length of the flame was longer for the rich mixtures. This lengthening of the flame allowed a greater residence time for the flame which increased the production of NO. This will be supported by Fig 4.4.4 discussed later.

**4.4.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** For a constant burner jet exit velocity of 20 m/s with varying equivalence ratio (Figures 4.4.1a and b), the 3:1 AR elliptical burner and the circular burner produced similar CO and NO emission indexes. However for CO, at an equivalence ratio of 0.55, the circular burner produced 0.73 g of CO per kg of fuel while the 3:1 AR elliptical burner produced 1.58 g/kg. This increase of CO is likely tied to the slight bifurcation seen at this condition, indicating localized quenching occurring at the premixed flame tip. Since the flames of the 3:1 AR elliptical and circular burner had similar flame lengths, the NO emission index would be expected to be similar (due to similar residence times) which is what is

shown. Overall, at laminar conditions, the circular and 3:1 AR elliptical burners were very similar in emission generation, thus the ellipticity of the burner showed little effect.

The emission results for an equivalence ratio held constant at 2.0 with varying burner exit Reynolds number are shown in Figures 4.4.2a and b. For the range of Reynolds number of 2000 to 6000, the circular and 3:1 AR elliptical burners produced similar CO production. At a Reynolds number of 7500, CO production was characterized by a great increase (over 300%) for the 3:1 AR elliptical burner while there existed only a moderate increase of 89% for the circular burner. For the 3:1 AR elliptical burner, there was a general decrease in NO production with an increase in Reynolds numbers. However, for the circular burner, there was a sharp decrease in NO in the range of Reynolds numbers of 2000 to 8000. NO production was higher for the circular burner in the range of Reynolds numbers of 6000 to 8000 and was similar to or lower than for the 3:1 AR elliptical burner NO production for Reynolds numbers of 2000 to 4000.

These results can be explained by the 3:1 AR elliptical burner transitioning to turbulence earlier than the circular burner with the resultant lowering of flame length reducing the residence time. For the condition of an equivalence ratio of 2.0, the transition to turbulence (with the subsequent increase in mixing rate) caused quenching in the 3:1 AR elliptical burner flame, thus the high CO production.

For equivalence ratio held constant at 4.0 with varying burner exit Reynolds number (Figure 4.4.3a and b), CO production generally increased with increasing Reynolds number and NO generally decreased with increase in Reynolds number for the circular and 3:1 AR elliptical burners. At Reynolds numbers less than 3000 the circular
and 3:1 AR elliptical burners produced similar NO and CO. However, the 3:1 AR elliptical burner tended to produce more CO and less NO than the circular burner at Reynolds numbers greater than 3000. This trend was more pronounced at higher Reynolds numbers.

The general trends of the data can be explained by the relative differences between initiations of transition to turbulent combustion. It can be seen that the increase of CO production due to the transition to a turbulent flame was much lower for an equivalence ratio of 4.0 than it was for the case of equivalence ratio of 2.0. At an equivalence ratio of 4.0, the enhanced mixing provided by transition to turbulence very likely did not lower the local equivalence ratio past the limits of flammability, thus allowing the combustion to proceed without quenching. Less CO was then created.

**4.4.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:** For a constant velocity of 20 m/s with varying equivalence ratio (Figs 4.4.1 a and b), the 4:1 AR elliptical burner produced more CO and less NO than the 3:1 AR elliptical burner.

At a fixed equivalence ratio of 2.0 with varying Reynolds number (Figs. 4.4.2 a and b), the 4:1 AR elliptical burner produced greater CO emissions than the 3:1 AR elliptical burner at an equivalence ratio of 5700 but had similar CO emissions for the other Reynolds numbers. The 4:1 AR elliptical burner produced less NO than the 3:1 AR elliptical burner over the range of Reynolds numbers tested.

At a fixed equivalence ratio of 4.0 (Figures 4.4.3a and b), for Reynolds numbers greater than 3000, the 3:1 AR elliptical burner produced greater CO than the 4:1 AR

elliptical burner. For Reynolds numbers less than 3000, the 4:1 AR elliptical burner produced greater CO than the 3:1 AR elliptical burner. NO emissions were greater for the 3:1 AR elliptical burner for Reynolds numbers of less than 6000 and were greater for the 4:1 AR elliptical burner for higher Reynolds numbers.

For varying Reynolds number with fixed equivalence ratio of 2.0, the 4:1 AR elliptical burner had a great increase in CO production at a Reynolds number of 5700, while the 3:1 AR elliptical burner had this dramatic jump in CO production later at a Reynolds number of 7600. For the circular to 3:1 AR elliptical burner comparison, this jump in CO production was linked to the flames transitioning to turbulence. However, from Fig. 4.3, we see that the 4:1 AR elliptical burner transitioned to a turbulent flame later than the 3:1 AR elliptical burner, opposite to what was seen with the CO production. The discrepancy is explained because the 4:1 AR elliptical burner had an overall enhanced mixing independent of the turbulence of the flame, which made the flame more sensitive to equivalence ratio reductions thus, the early increase in CO production compared to the 3:1 AR elliptical burner. A comparison of results at the fixed equivalence ratio of 2.0 to the fixed equivalence ratio of 4.0 confirms this analysis. Since it is unlikely that the equivalence ratio of 4.0 flame will be lowered past the lean flammability limits, we would expect the 4:1 AR elliptical and 3:1 AR elliptical burners not to exhibit this drastic increase in CO production. Figure 4.4.3a shows that this drastic increase did not occur. NO production is again linked to the flame length with shorter flames producing lower NO.

Figure 4.4.4 shows the effects of flame length on the nitric oxide emission index. It can be seen that the NO emission index was a strong function of flame length (thus residence time) for all three burners with increasing NO emission index with increasing flame length. This was as expected (Turns and Myhr (1991), Turns et al. (1993), and Lyle et al. (1999)). Interesting however, was the observation that the 4:1 AR elliptical burner, for a given flame length, tended to produce greater NO emission index than the circular and 3:1 AR elliptical burners. The velocity decay exhibited by the 4:1 AR elliptical burner decreases the bulk velocity of the flame, thus allowing a greater residence time even with a shorter flame length.

## 4.5: Radiative Fraction

**4.5.1 General Observations:** From Figures 4.5.1a and b, there was no significant difference in the radiative fraction when the flame was viewed normal to the major or minor axis of the burners. Since there were no major differences between major and minor axes, only the major axis results will be presented for the following.

Examining Figs. 4.4.2a and b, it can be seen that the radiative fraction decreased with increased Reynolds number. This behavior was also seen in the visual intensity of the flame.

**4.5.2 Effect of Level of Premixing:** Examining Fig. 4.5.1a, for the circular and 3:1 AR elliptical burners, for the range of equivalence ratios of 2.0 to 4.0, the radiative fraction was relatively constant, with a slight increase with increase in equivalence ratio. This increase could be due to a small increase in the free carbon in the system (since premix air is decreased) causing a small increase in continuum radiation from soot.

For an equivalence ratio of 1.0, there was a slight increase in the radiative fraction compared to equivalence ratios of 2.0 to 4.0. However, an equivalence ratio of 0.55 had a radiative fraction double that of the range of equivalence ratios of 2.0 to 4.0. This is in contrast to what was seen with the flame images. There, the flame for an equivalence ratio of 1.0 had the brightest appearance.

As will be seen in the spectral analysis of the flames, the increased radiative fraction of the equivalence ratio of 0.55 flame is due to a much greater percentage of energy being released at 306 nm for the lean flame compared to the richer flames. Since the 306 nm was not visible, this increase would not be seen in the flame images.

The 4:1 AR elliptical burner had a fairly constant radiative fraction with change in equivalence ratio with only slight increase seen at an equivalence ratio of 0.55 and 4.0.

**4.5.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** For the fixed velocity varying equivalence ratio case (Fig. 4.5.1a), the circular and 3:1 AR elliptical burners produced similar radiative fractions for all conditions. For a fixed equivalence ratio of 2.0 with varying Reynolds number (Fig. 4.5.2a), the circular and 3:1 AR elliptical burner produced nearly identical radiative fractions. For a fixed equivalence ratio of 4.0 (Fig. 4.5.2b), the circular burner had a slightly lower radiative fraction than the 3:1 AR elliptical burner for Reynolds numbers greater than 5000.

**4.5.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:** For most conditions, the difference between the radiative fraction between the 3:1 AR elliptical burner and the 4:1 AR elliptical burner was small. However, at a constant velocity of 20 m/s and equivalence ratio of 0.55 the 4:1 AR elliptical burner radiative fraction was 46.9% lower than with the 3:1 AR elliptical burner. The 4:1 AR elliptical burner also produced a 23% lower radiative fraction than the 3:1 AR elliptical burner at an equivalence ratio of 1.0 This was due to the splitting of the 4:1 AR elliptical burner flame and the subsequent reduction of radiative emission area.

No significant difference was seen between the 3:1 AR elliptical and 4:1 AR elliptical burner flames for varying Reynolds number at a constant equivalence ratio of 2.0. For an equivalence ratio of 4.0, the 4:1 AR elliptical burner produced slightly higher radiative fraction than the 3:1 AR elliptical burner results. The enhanced mixing

of the 4:1 AR elliptical burner allowed, for the primarily diffusion flame characteristics of the rich air/fuel mixture, an effectively lower equivalence ratio than the 3:1 AR elliptical burner and thus radiated more energy.

## 4.6: Radiation Wavelength Spectra

**4.6.1 General Observations:** Measurements were taken at two flame height locations, 75% of the length of the premixed zone of the flame and at a height of 50% of the overall flame length. This allowed a comparison of the premixed flame zone radiative emissions and the diffusion flame zone radiative emissions giving an indication of the global combustion processes occurring at those heights. The emissions were scanned from the near ultraviolet (200 nm) to the red region (600 nm) of the spectrum. This range of wavelengths allowed the detection of many chemilumensent species of combustion interest.

There were eight observable emission peaks and peak pairs seen for the test conditions (Figs. 4.6.1a through 4.6.7c) and these eight peaks were produced by three chemiluminesent species:  $OH^*$ ,  $CH^*$  and  $C_2^*$ . Relevant emission characteristics for these species are given in Table 4.6.1. The slash-listed wavelengths are where the species peaks were too close in wavelength and/or were of too low intensity to effectively resolve, so they appeared as a single peak or closely spaced double peaks. There was a region of mild continuum radiation from 260 to 500 nm with a peak at about 365 nm.

Both the species peaks and the continuum radiation were qualitatively similar to that seen with the study from Kojima, et al (2000), however the current study produced much greater OH<sup>\*</sup> radiation due to the use of hydrogen for flame anchoring. The Kojima et al study used methane for the fuel. To ease the comparison of relative emissions of the chemiluminescent species, the radiative emissions were normalized to the magnitude of the strong OH<sup>\*</sup> peak located at 306 nm. The measured signal for the OH<sup>\*</sup> is reported in the figures. The reported signal is the voltage output for the OH<sup>\*</sup> peak for that scan. The

excitation voltage of the photomultiplier tube was held constant for all measurements so the voltage of each condition should be proportional to the radiative output. OH<sup>\*</sup> was present for all conditions so it gives a convenient normalization criterion.

For all tested conditions, the  $OH^*$  emission peak was dominant. The premixed region of the flame (75% of bright blue height) had much greater  $OH^*$  emission, up to 20 times greater, compared to the non-premixed zone of a particular flame.  $CH^*$  and  $C_2^*$  emissions were, for the majority of cases, only detected in the premixed region and had magnitudes much smaller than that of  $OH^*$  indicating that the majority of fuel decomposition reactions (as indicated by the presence CH and C<sub>2</sub>) are occurring in the premixed zone. The lack of  $CH^*$  and  $C_2^*$  in the dim outer envelope of the flame supports the suggestion that this region does not have significant decomposition of unburned fuel components and soot for the equivalence ratios tested.

**4.6.2 Effect of Level of Premixing:** Looking at the effects of varying premixing of radiative emissions, at the premixed zone of the flame increased equivalence ratio caused a decrease in  $OH^*$  radiative intensity and an increase in the intensity of the  $CH^*$  and  $C_2^*$  emission lines. For the non-premixed zone of the flame, an increase in equivalence ratio caused an increase in the OH radiative emission intensity. These observations were seen for all cases except for the 4:1 AR elliptical burner at an equivalence ratio of 0.55 which will be discussed in section 4.6.4.

With increased equivalence ratio, it would be expected the decrease in oxygen present in the fuel air jet would reduce the intensity of the reactions in the premixed flame region and increase the amount of unburned fuel components passing through the premixed flame zone. This behavior was seen in the decrease of  $OH^*$  emission intensity at the premix flame region and in the greater proportion of  $CH^*$  and  $C_2^*$  emissions in the flame.

**4.6.3 Comparison of Circular to 3:1 Aspect Ratio Elliptical Burners:** The 3:1 AR elliptical burner and the circular burner have very similar radiative emission profiles both in OH<sup>\*</sup> magnitude and relative peak intensities. However, for the lean flame, in the non-premixed zone, the OH<sup>\*</sup> intensity is half that of the circular burner for the 3:1 AR elliptical burner. For the premixed zone at an equivalence ratio of 0.55, the ellipticity of the burner does not seem to change radiative emissions. This decrease in OH<sup>\*</sup> in the 3:1 AR elliptical burner mirrors the increase in CO emissions for the equivalence ratio of 0.55 flame. It appears that the combustion intensity of the diffusion flame of the 3:1 AR elliptical burner (as indicated by the OH<sup>\*</sup> radiation) was reduced which allowed more CO to escape complete combustion.

**4.6.4 Comparison of 4:1 Aspect Ratio Elliptical and 3:1 Aspect Ratio Elliptical Burners:** In the premixed flame zone, for an equivalence ratio of 0.55, the 4:1 AR elliptical burner has similar peak intensities for OH\* and similar relative peaks intensities for CH<sup>\*</sup> and C<sub>2</sub><sup>\*</sup> as seen with the 3:1 AR elliptical burner. For the moderately rich flame condition of equivalence ratio of 2.0, the 4:1 AR elliptical burner had significantly greater OH<sup>\*</sup> radiation than the 3:1 AR elliptical burner (49.7% greater than 3:1). The CH<sup>\*</sup> and C<sub>2</sub><sup>\*</sup> peaks were also higher for the 4:1 AR elliptical burner relative to what was observed with the 3:1 AR elliptical burner. The shorter flame of the 4:1 AR elliptical burner leads to an increased reaction rate which, for a constant fuel input, implies a greater amount of fuel decomposition species at the premixed flame.

In the diffusion zone, for an equivalence ratio of 0.55, the 4:1 AR elliptical burner has much higher OH<sup>\*</sup> emission than the 3:1 burner (17.6 times greater). In addition, unlike the 3:1 AR elliptical burner, a small amount of CH<sup>\*</sup> radiation is seen for the 4:1 AR elliptical burner. Due to the small scale of the 4:1 AR elliptical burner at lean conditions, this was likely some bleed through of light emitted from the premixed zone into the diffusion flame spectra. For the equivalence ratio of 2.0 flame, similar to the 3:1 AR elliptical burner flame spectra, only a strong OH<sup>\*</sup> peak structure was seen with the 4:1 AR elliptical burner. No other chemiluminesent species peaks were observed. The OH<sup>\*</sup> intensity of the 4:1 AR elliptical burner was 35% greater than that of the 3:1 AR elliptical burner. For an equivalence ratio of 4.0, again, only a strong OH<sup>\*</sup> signal was seen with the 4:1 AR elliptical burner in the diffusion zone of the flame. The 3:1 AR elliptical burner, however, had a small amount of CH<sup>\*</sup> species. The OH<sup>\*</sup> intensity of the 4:1 AR elliptical burner was 9.2% lower than that of the 3:1 AR elliptical burner.

## 4.7: Chapter Conclusions

The following conclusions can be drawn regarding the global properties of premixed flames from elliptical burners.

Increasing the hydrogen mass fraction of the hydrogen/propane fuel mixture resulted in increased blowout velocity for the flames. For a hydrogen percentage of 40% by mass in propane, at burner exit equivalence ratios of less than 1.0, the maximum blowout velocities for the circular, 3:1 AR elliptical, and 4:1 AR elliptical burners, were similar. At a burner exit equivalence ratio of 1.0 and greater, the circular burner was able to attain a higher blowout velocity than both the 3:1 AR and 4:1 AR elliptical burners. Between the elliptical burners, where there was a difference, the 4:1 AR elliptical burner had a greater blow out velocity than the 3:1 AR elliptical.

Transition to a turbulent flame occurred at the highest Reynolds number of the three burners for the circular burner. Elliptical burners are known to exhibit higher turbulence levels than circular burners, thus this difference is expected. The 3:1 AR elliptical burner tended to transition from a laminar to a turbulent flame at a lower Reynolds number than the 4:1 AR elliptical burner. The 4:1 AR elliptical burner flame has an increased velocity decay rate that reduces the turbulence generation, thus the flame becomes turbulent at a greater velocity than the 3:1 AR elliptical burner. The critical Reynolds number of the circular burner increased with an increase in the burner exit equivalence ratio while the elliptical burner's critical Reynolds number was insensitive to an increase in equivalence ratio.

The flames of this study consisted of two visual regions: a bright blue inner cone corresponding to a premixed flame and a dim bluish outer flame corresponding to a

diffusion type flame. The diffusion flame consisted of the uncompleted reactions exiting the premixed flame.

At a burner jet exit velocity of 20 m/s, the flames were laminar and the circular and 3:1 AR elliptical burners were similar in appearance and overall flame length for lean to rich equivalence ratios. For these conditions, the 4:1 AR elliptical burner split into two sub-flames along the burner major axis. This splitting greatly shortened the 4:1 AR elliptical flame to have about half the overall and premixed region flame length as that of the circular and 3:1 AR elliptical flames. The length of both the premixed and diffusion flame regions increased with increasing burner exit equivalence ratio for the three burners.

Varying the burner exit Reynolds number while fixing the equivalence ratio to 2.0 resulted in the elliptical burners having a shorter overall flame length than the circular burner for Reynolds numbers greater than 3000. The 4:1 AR elliptical burner had an overall flame length of approximately half that of the 3:1 AR elliptical burner over the range of Reynolds numbers. The circular burner increased slightly in overall flame length with increase in Reynolds number while the elliptical burners overall flame length remained constant. The premix flame region had similar flame lengths for the 3:1 AR elliptical numbers greater than 4000, the circular burner developed a longer premixed flame length. The circular and 3:1 AR elliptical burners premix flame increased in length with increase in Reynolds number for premixed flame length at a solution of 7600 where the premixed length showed a slight increase.

With a fixed equivalence ratio of 4.0 with varying Reynolds numbers, the overall flame lengths of the 3:1 AR elliptical and circular burners were similar for burner exit Reynolds numbers of 1600 to 3200; both increased in length with increase of jet exit Reynolds number. For Reynolds numbers greater than 3200, both the circular and 3:1 AR elliptical burners began to decrease in overall flame length with increase in Reynolds number (as they transitioned from laminar to turbulent), however, the 3:1 AR elliptical burner flame length decreased at a much faster rate than the circular burner flame length. The 4:1 AR elliptical overall flame length was constant for varying Reynolds numbers for the rich equivalence ratio of 4.0 and was lower than the flame length of the circular and 3:1 AR elliptical burners for Reynolds numbers less than 4700. At a Reynolds number of 7900, the overall flame length of the three burners was similar.

In the laminar flames of this study, the 3:1 AR elliptical and circular burners produced similar carbon monoxide and nitric oxide emission indexes over a range of equivalence ratios of 0.55 to 4.0. The 4:1 AR elliptical burner produced greater CO and lower NO emission indexes than the other two burners for laminar flames. For all burners an increase in equivalence ratio tended to decrease the production of CO and increase the production of NO.

With an increase in jet exit Reynolds number resulting in turbulent flames, both the elliptical burners tended to produce more CO and less NO than the circular burner, with the difference between the elliptical and circular burner emission production being greatest at an equivalence ratio of 2.0.

In Chapter 5, the fundamental processes producing the above behavior will be explored and will be used to explain and support the above observations.

Jet Exit Velocity (m/s)	Jet Exit Equivalence Ratio	Cold Jet Reynolds Number
20	0.55	2310
20	1.0	2150
20	2.0	1900
20	3.0	1730
20	4.0	1600
40	2.0	3780
40	3.0	3440
40	4.0	3190
60	2.0	5620
60	3.0	5100
60	4.0	4720
80	2.0	7500
80	3.0	6860
80	4.0	6360
100	3.0	8570
100	4.0	7950

Table 4.1.1: Reynolds Numbers for Jet Conditions

Table 4.6.1: Major Radiative Emission Species

Emission Wavelength	Species	Transistion
281.1	OH	$A^{2}\Sigma^{+}$ - $X^{2}\Pi_{i}(1,0)$
306.4	OH	$A^{2}\Sigma^{+}$ - $X^{2}\Pi_{i}(0,0)$
387.1	СН	$B^{2}\Sigma^{-} - X^{2}\Pi(0,0)$
431.4	СН	$A^{2}\Delta - X^{2}\Pi(0,0)$
438.2	$C_2$	$A^{3}\Pi_{g}$ - $X^{3}\Pi_{u}$ (2,0) VW
471.5/473.7	$C_2$	$A^{3}\Pi_{g} - X^{3}\Pi_{u}(2,1)/(1,0)$
512.9/516.5	$C_2$	$A^{3}\Pi_{g}$ - $X^{3}\Pi_{u}(1,1)/(0,0)$
558.5/563.6	$C_2$	$A^{3}\Pi_{g}$ - $X^{3}\Pi_{u}(1,2)/(0,1)$



Figure 4.1.1a: Blowout Stability Limit for Circular Burner (Maximum Jet Velocity Attainable)



Figure 4.1.1b: Blowout Stability Limit for 3:1 Aspect Ratio Elliptical Burner (Maximum Jet Velocity Attainable)







Figure 4.1.1d: Blowout Stability Limit for Circular Burner (Maximum Reynolds Number Attainable)



Figure 4.1.1e: Blowout Stability Limit for 3:1 Aspect Ratio Elliptical Burner (Maximum Reynolds Number Attainable)



Figure 4.1.1f: Blowout Stability Limit for 4:1 Aspect Ratio Elliptical Burner (Maximum Reynolds Number Attainable)



Equivalence Ratio of Premixed Jet

Figure 4.1.2a: Partial Liftoff Limit for Circular Burner (Maximum Jet Velocity Attainable)



Figure 4.1.2b: Partial Liftoff Limit for 3:1 Apect Ratio Elliptical Burner (Maximum Jet Velocity Attainable)



Figure 4.1.2c: Partial Liftoff Limit for 4:1 Aspect Ratio Elliptical Burner (Maximum Jet Velocity Attainable)







Figure 4.1.2e: Partial Liftoff Limit for 3:1 Apect Ratio Elliptical Burner (Maximum Reynolds Number Attainable)



Figure 4.1.2f: Partial Liftoff Limit for 4:1 Aspect Ratio Elliptical Burner (Maximum Reynolds Number Attainable)



Figure 4.1.3 Transition from Laminar to Turbulent for 40% by Mass Hydrogen in Propane Mixture







Figure 4.2.1b: Major Axis Flame Appearance of 3:1 Aspect Ratio Elliptical Burner with Varying Premix Equivalence Ratio at a Burner Jet Exit Velocity of 20 m/s.



Figure 4.2.1c: Minor Axis Flame Appearance of 3:1 Aspect Ratio Elliptical Burner with Varying Premix Equivalence Ratio at a Burner Jet Exit Velocity of 20 m/s.







Figure 4.2.1e: Minor Axis Flame Appearance of 4:1 Aspect Ratio Elliptical Burner with Varying Premix Equivalence Ratio at a Burner Jet Exit Velocity of 20 m/s.







Figure 4.2.2b: Major Axis Flame Appearance of 3:1 Aspect Ratio Elliptical Burner with Varying Burner Jet Exit Reynolds Number at a Premix Equivalence Ratio of 2.0.



Figure 4.2.2c: Minor Axis Flame Appearance of 3:1 Aspect Ratio Elliptical Burner with Varying Burner Jet Exit Reynolds Number at a Premix Equivalence Ratio of 2.0.



Figure 4.2.2d: Major Axis Flame Appearance of 4:1 Aspect Ratio Elliptical Burner with Varying Burner Jet Exit Reynolds Number at a Premix Equivalence Ratio of 2.0.



Figure 4.2.2e: Minor Axis Flame Appearance of 4:1 Aspect Ratio Elliptical Burner with Varying Burner Jet Exit Reynolds Number at a Premix Equivalence Ratio of 2.0.



Figure 4.2.3: Axis Switching in 3:1 AR Elliptical Burner at an Equivalence Ratio of 2.0 with Varying Reynolds Number



Figure 4.3.1a: Normalized Overall Flame Length for Varying Premix Equivalence Ratio at Burner Jet Exit Velocity 20 m/s



-igure 4.3.1 b: Normalized Premixed Region Flame Length for Varying Premix Equivalence Ratio at Burner Jet Exit Velocity 20 m/s











Equivalence Ratio of 4.0 with Varying Burner Jet Reynolds Number



Figure 4.4.1a: CO Emissions for Varying Premix Equivalence Ratio at Burner Jet Exit Velocity of 20 m/s



Figure 4.4.1b: NO Emissions for Varying Premix Equivalence Ratio at Burner Jet Exit Velocity of 20 m/s



Figure 4.4.2a: CO Emissions for Premixed Equivalence Ratio of 2.0 with Varying Burner Jet Exit Reynolds Number



Figure 4.4.2b: NO Emissions for Premixed Equivalence Ratio of 2.0 with Varying Burner Jet Exit Reynolds Number



Figure 4.4.3a: CO Emissions for Premixed Equivalence Ratio of 4.0 with Varying Burner Jet Exit Reynolds Number



Figure 4.4.3b: NO Emissions for Premixed Equivalence Ratio of 4.0 with Varying Burner Jet Exit Reynolds Number



Figure 4.4.4: NO Emissions Scaled to Flame Length



Figure 4.5.1a: Variation of Major Axis Radiative Fraction with Change in Equivalence Ratio and Burner Geometry for Burner Jet Exit Velocity of 20 m/s



Jet Exit Velocity of 20 m/s



Figure 4.5.2a: Variation of Major Axis Radiative Fraction with Change in Burner Jet Exit Reynolds Number and Burner Geometry for Equivalence Ratio of 2.0








Figure 4.6.2c: Spectral Emissions for 4:1 Aspect Ratio Elliptical Burner at 75% Premixed Region Flame Length for 20 m/s Jet Exit Velocity and 2.0 Equivalence Ratio



Figure 4.6.3c: Spectral Emissions for 4:1 Aspect Ratio Elliptical Burner at 50% Overall Flame Length for 20 m/s Jet Exit Velocity and 0.55 Equivalence Ratio



Figure 4.6.4c: Spectral Emissions for 4:1 Aspect Ratio Elliptical Burner at 50% Overall Flame Length for 20 m/s Jet Exit Velocity and 2.0 Equivalence Ratio



and 4.0 Equivalence Ratio



Figure 4.6.6c: Spectral Emissions for 4:1 Aspect Ratio Elliptical Burner at 75% Premixed Region Flame Length for 60 m/s Jet Exit Velocity and 2.0 Equivalence Ratio



Burner at 50% Overall Flame Length for 60 m/s Jet Exit Velocity and 2.0 Equivalence Ratio

## **CHAPTER 5: FLAME STRUCTURE**

Traverse profiles of the measured quantities were taken at heights of 12.5% (nearburner), 25% (midflame), and 50% (far-flame) of the total flame length of the tested flame (Table 5.1). At a flame height of 12.5%, the profile passed through the premix flame and at 50% the profile consisted of the diffusion type flame. The midflame (25%) corresponded roughly with the transition of the flame from the premix to diffusion type flame. Thus, these flame heights were representative of the processes occurring within the flame and gave a comparison on how the processes differ between burners.

To examine the effect that equivalence ratio has on laminar flames issuing from elliptic burners, profiles were taken for equivalence ratios of 0.55, 1.0, 2.0, and 4.0 at a burner bulk jet exit velocity of 20 m/s. This has a range of Reynolds numbers of 2300 at an equivalence ratio of 0.55 and 1600 at an equivalence ratio of 4.0. Major axis profiles were taken for all burners and equivalence ratios. Minor axis profiles were taken for equivalence ratios of 1.0 and 4.0 for the 3:1 AR elliptical burner. Minor axis profiles were not taken for the 4:1 AR elliptical burner due to its splitting.

Profiles were also taken for a turbulent flame with a jet exit velocity of 100 m/s at an equivalence ratio of 4.0. This corresponded to an exit Reynolds number of 7950. The primary focus is given to the laminar flames of the study, however, a comparison of the behavior of the turbulent flames to the laminar cases will be given at the end of each section. The high velocity of these flames were not able to be reliably measured with the PDPA system used for this study, therefore velocity profiles are not given. Profiles of velocity, temperature, and concentration were symmetric, within the experimental uncertainty, about the centerline along the major and minor axis, thus only half of the transverse distributions are shown in the figures.

#### 5.1: Flow Field

# 5.1.1 Velocity:

**5.1.1.1 General Observations:** Measurements of velocity were taken using a Phase Doppler Particle Analyzer (PDPA) with the air component of the burner fuel/air mixture seeded with magnesium oxide particles as was described in Section 3.2.4. Since PDPA requires the presence of seed particles, it follows that velocity measurements were taken only where sufficient seed particles were present to be read by the instrumentation. This leads to many of the reported velocity profiles not reaching zero velocity at the edge of the flame. The lack of seed particles near the flame edges could be due reduced seed particle transfer to the edge of the flame particularly for the laminar flames.

The laminar flame conditions reported in Figs. 5.1.1a to 5.1.5f were produced with a reacting 40% by mass H<sub>2</sub>/propane mixture for equivalence ratios of 0.55, 1.0, 2.0, and 4.0 and a jet exit velocity of 20 m/s (Re = 1600 to 2300). The turbulent flames shown in Figures 5.1.5a to f were a 40% by mass H<sub>2</sub>/propane mixture with an equivalence ratio of 4.0 with a jet exit velocity of 100 m/s (Re = 7950). For safety considerations, the cold jet data were produced using only air as the jet fluid. This was reasonable due to the high proportion of air in the premixed jets. For the cold jets, profiles were taken at the same locations above the burner as in the flames.

Figures 5.1.1a to 5.1.1f show that the laminar flames had a higher measured maximum axial velocity than the cold jets at a given height, particularly at the higher axial locations. This higher velocity was expected since the heating provided by combustion caused gas expansion which increased the flow velocity. Also, the heating of the gas decreased the turbulence level of the combusting jet (as will be shown in

subsequent figures) which reduced the velocity decay of the jet both through reduction of momentum transfer to the quiescent and in the reduction of internal flow losses. The 3:1 AR elliptical burner had a much higher maximum velocity magnitude than the circular and 4:1 AR elliptical burners. The 3:1 AR elliptical burner exhibited increased heating of the core due to increased flame circumference and closer proximity of the flame fronts on the minor axis (as will be shown in the schlieren images (Section 5.2)). This increased the velocity through increased gas expansion. The 4:1 AR elliptical burner also had an increased flame circumference, but had a greater velocity decay rate due to splitting which counteracted the increased gas expansion.

For the cold jets corresponding to the laminar flames, (Figs. 5.1.1d to f) with the circular and 3:1 AR elliptical burners, there was a region of near constant maximum axial jet velocity to a  $x/d_{eff}$  of 10. This was consistent with the presence of a potential core for the cold jet. The maximum axial velocity then decreased with increasing axial distance. The 4:1 AR elliptical burner did not exhibit the region of constant maximum axial velocity with increasing axial distance for the cold jet. This was likely a side effect of the splitting of the flame disrupting the potential core by increasing shear through the large increase of circumference area.

For laminar flame conditions, there was more scatter in the velocity data (due to variation in local equivalence ratio leading to changes of the flame properties). A potential core was apparent for all three burners and was longer than the burners' cold jet potential core. The 3:1 AR elliptical burner had a longer potential core than the circular burner. This core existed to an axial distance of 20  $x/d_{eff}$  for the 3:1 AR elliptical burner

compared to axial distance of 15  $x/d_{eff}$  for the circular burner. The 4:1 AR elliptical burner exhibited a potential core to an axial distance of 8  $x/d_{eff}$ .

In the velocity decay region, the velocity tended to decrease less with increase in axial distance for the laminar flame compared to that of the cold jet. Both the extension of the potential core and the reduction of velocity decay were due to the presence of the flame reducing the mixing of the flame (through the increase in gas viscosity) thus reducing the momentum transfer of the jet to the surrounding quiescent air. It would appear that the 3:1 AR elliptical burner had a lengthened potential core compared to the circular due to the greater heating of the core flow. This greater heating of the core allows the laminar core to exist to longer lengths through increase in viscosity with a contribution from the increased velocity of the 3:1 AR elliptical burner flow adding momentum.

**5.1.1.2 Effect of Level of Premixing:** While examining the radial profiles of axial velocity of the laminar flames (Figs. 5.1.2a to 5.1.5l) for equivalence ratios of 1.0 and greater with a combusting jet, it was noticed that increasing the equivalence ratio tended to decrease the half width of the velocity profile (defined as the radial distance where the axial velocity decreased to 50% of the profile maximum) at the near-burner region for the circular burner and the 3:1 AR elliptical burner. The midflame and far-flame profiles showed nearly constant velocity width with increasing equivalence ratio for the circular and 3:1 AR elliptical burners.

This was due to the reduction of the spreading rate from the presence of the flame. The cold jet profile's velocity half width increased with increasing equivalence ratio. With increase in equivalence ratio, the profiles were taken at increasing distances from the burner, thus the wider profiles for the cold jet. The 4:1 AR elliptical burner showed an increasing velocity profile width for all conditions, which is a result of the angle of the splitting of the jet.

At equivalence ratios of 0.55 and 1.0, in the laminar circular and 3:1 AR elliptical burners at the near-burner, the flame velocity distribution was wider than the velocity distribution of the corresponding cold jet. At an equivalence ratio of 2.0, the 3:1 AR elliptical burner had similar reacting and cold jets flame widths. The circular cold jet was narrower than the reacting jet at these conditions. Finally, at an equivalence ratio of 4.0, the flame had a narrower velocity profile than the cold jet for both the 3:1 AR elliptical and circular burners.

For the midflame and far-flame profiles, the velocity half width of the cold jet was narrower than the flame for the circular and 3:1 AR elliptical burners for a lean equivalence ratio of 0.55. At an equivalence ratio of 1.0, the midflame profile widths for the cold and flame conditions were similar, but, at the far-flame, the flame profile was narrower than that of the cold jet for the circular and 3:1 AR elliptical burners. In flames with equivalence ratio of 2.0 and greater, the midflame and far-flame profiles were wider for the cold jet than for the flame.

The reacting jet produced a much lower RMS of the velocity than the cold jet at the midflame and far-flame regions of equivalence ratios of 1.0 to 4.0 with the difference in RMS of the velocity between cold jet and flame jet increasing with increase in equivalence ratio. The RMS of the velocity was similar between the burners at the nearburner and mid burner for an equivalence ratio of 0.55. For the laminar flames with equivalence ratios of 0.55 and 1.0, the maximum normalized RMS of the velocity decreased with increase in axial distance for the three burners with the exception of the 4:1 AR elliptical burner at an equivalence ratio of 0.55, where the RMS of the velocity increased from the near-burner to midflame. This increase in the RMS of the velocity for the 4:1 AR elliptical burner was likely due to the transition from a single jet to the split jet.

At an equivalence ratio of 2.0, the 3:1 AR elliptical burner showed an increase in maximum normalized RMS of the velocity from the near-burner region to the midflame position. The 4:1 AR elliptical burner's RMS of the velocity remained constant while the circular burner had a decrease in the maximum normalized RMS of the velocity from the near-burner to midflame. From the midflame to the far-flame heights, the circular burner increased its maximum normalized RMS of the velocity and the 3:1 AR elliptical and 4:1 AR elliptical burners decreased slightly.

For an equivalence ratio of 4.0, the circular burner exhibited a decrease in maximum normalized RMS of the velocity and the 3:1 AR elliptical and 4:1 AR elliptical burners had similar maximum normalized RMS of the velocity from the near-burner to the midflame. The 3:1 AR elliptical and 4:1 AR elliptical burners decreased in maximum normalized RMS of the velocity from the midflame to far-flame position while the circular burner increased.

The presence of a flame reduces the mixing of a jet (as exhibited in the reduction of the RMS of the velocity) through the general tendency of heated jets to become laminar. This reduces the width of the flame velocity profile due to inhibition of momentum transfer between the jet and the ambient air. The higher flame temperatures of a stoichiometric to rich mixture compared to a lean mixture (as will be seen in Section 5.2) allowed the gas jet to remain laminar longer than the cold jet. This reduced the spreading rate.

**5.1.1.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** Figures 5.1.1a and b show that the laminar flames of the 3:1 AR elliptical burner had a higher maximum flame gas velocity compared to the circular burner at all flame locations and equivalence ratios. The cold jet (Figs. 5.1.1d and e) exihibited similar maximum axial velocities for the circular and 3:1 AR elliptical burners. The difference in behavior between the cold and reacting jets is likely due to the increased circumferential area of the 3:1 AR elliptical burner allowing a greater heat transfer from the flame boundary to the core of the flame, thus increasing the gas expansion.

For several of the 3:1 AR elliptical burner and circular burner laminar flame axial velocity profiles (Figs. 5.1.2a to f, 5.1.3a to f, 5.1.4a to f, and 5.1.5a to f), a region of constant velocity was seen about the centerline. The 3:1 AR elliptical and circular burners both showed a region of constant velocity for the near-burner profiles for equivalence ratios of 0.55 and 1.0 and at the midflame for an equivalence ratio of 0.55. The 3:1 AR elliptical burner had additional regions of constant velocity at the near-burner for equivalence ratios of 2.0 and 4.0 and the midflame of equivalence ratios of 1.0 and 2.0. The far-flame velocity profiles did not show the constant velocity behavior for either burner.

In the laminar flame with an equivalence ratio of 0.55, for the 3:1 AR elliptical burner, the constant velocity width increased from the near-burner to the midflame

profile, but at all other equivalence ratios the constant velocity width decreased with increase in axial distance. A mild double peak type structure could be seen for the near-burner equivalence ratio of 1.0 for the 3:1 AR elliptical burner.

For the cold jet, the 3:1 AR elliptical burner had a core of constant velocity at the near-burner for equivalence ratios of 0.55, 1.0, and 2.0 and this core was seen for the midflame for an equivalence ratio of 0.55. For the midflame, at an equivalence ratio of 0.55 and the near-burner equivalence ratio of 1.0 and 2.0, there was a slight double peak structure seen in the cold jet velocity profiles for the 3:1 AR elliptical burner.

The region of constant velocities seen in the laminar flame profiles confirms the previous observations from in Section 5.1.1.1 concerning the presence of a potential core in the jets (since the region of constant velocity is one of the defining characteristics of a potential core). This core tended to last longer for flame conditions than in cold conditions (due to the laminarization of the jet) and for the 3:1 AR elliptical burner compared to the circular burner.

For the normalized RMS of the velocity (Figs. 5.1.2g to l, 5.1.3g to l, 5.1.4g to l, and 5.1.5g to l), the following trends were observed: for the laminar reacting jet, the maximum normalized RMS of the velocity for the 3:1 AR elliptical burner was greater than that of the circular burner for all flames, except for the far-flame profiles of equivalence ratio 1.0 and 2.0 where the maximum normalized RMS of the velocity was similar between the 3:1 AR elliptical and circular burners. The inherent instability which leads to enhanced turbulence generation) of the elliptical burners seen for cold jets (Crighton (1973), Ho and Gutmark (1987), Hussain and Husain (1989), and Miller, Madnia, and Givi (1995)) and diffusion flames (Gollahalli, Khanna, and Prabhu (1992),

Kamal (1995), Papanikolaou and Wierzba (2001), and Gollahalli and Pardivalla (2002)), is still present in premixed flames.

Examining the cold jet RMS of the velocity, the normalized maximum RMS of the velocity of the 3:1 AR elliptical burner was greater than that of the circular burner at the midflame for an equivalence ratio of 0.55 and at the near-burner and far-flame for an equivalence ratio of 2.0. The normalized cold jet RMS of the velocity was lower than in the circular burner for the 3:1 AR elliptical burner for the far-flame position for equivalence ratios of 1.0 and 4.0. All other tested flame heights had similar maximum RMS of the velocity for the two burners.

The shape of the normalized RMS of the velocity profiles of the 3:1 AR elliptical burner laminar flames correlated to the combusting velocity profiles for almost all flames. However, for the near-burner region of flames of equivalence ratios of 0.55 and 1.0, the normalized RMS of the velocity had a double peak structure with the peak normalized RMS of the velocity on the centerline side of the outside edge of the constant velocity region. This peak is a result of a shear interaction between the potential core and the quiescent environment. For all flame heights at an equivalence ratio of 4.0, there was an increase in the normalized RMS of the velocity on both sides of the region of radial rapid velocity decay.

The circular burner laminar flames exhibited the double peak of the normalized RMS of the velocity as seen in the 3:1 AR elliptical burner only for an equivalence ratio of 0.55. For the near-burner profile for equivalence ratios of 1.0 and 2.0 and the midflame position of equivalence ratio of 1.0, the RMS of the velocity tended to match

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the shape of the axial gas velocity for the circular burner. All other circular, reacting jet profiles of the RMS of the velocity were constant with radial position.

The axis switching that was previously observed for turbulent cold jets and flames was also seen in the laminar velocity profiles of this study. Comparing half width profiles, a definite axis switching (location where the half-width velocity profile along the minor axis was wider than the velocity profile along the major axis) was observed in the cold jet for equivalence ratio of 1.0 and 4.0 and in the flame condition of equivalence ratio of 4.0 with the switching occurring somewhere between the near-burner and midflame profiles. For an equivalence ratio of 1.0, at the midflame and far-flame, the velocity profiles of the major and minor axis were equal in half width. In turbulent flames, axis switching occurs due to instabilities created from the shedding of vortexes along the burner circumference. For laminar flames there is no such shedding. The mechanism for laminar flame axis switching is not clear.

**5.1.1.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:** The velocity measurements of the 4:1 AR elliptical burner laminar flame support the splitting of the flame as first observed in the flame images (Section 4.2.1). For the 4:1 AR elliptical burner with combustion (Figures 5.1.2a to c, 5.1.3a to c, 5.1.4a to c, and 5.1.5a to c), splitting, determined by significant peaks of velocity symmetric about the centerline on the major axis, was seen in the PDPA results for all flames except the near-burner and midflame regions of the equivalence ratio of 0.55 and the near-burner equivalence ratio of 1.0 flame. At those conditions, the velocity was either constant across the detectable region or only slight peaks in velocity were observed.

The cold jet ((Figures 5.1.2d to f, 5.1.3d to f, 5.1.4d to f, and 5.1.5d to f), exhibitied splitting at the near-burner for all equivalence ratios and at the midflame height for equivalence ratios of 0.55 to 2.0. The jets coalesced into a single velocity peak (located at the centerline) for the remaining flame heights and equivalence ratios. At the flame condition, the velocity peaks tended to diverge with increasing axial distance for all equivalence ratios greater than 0.55. At this fuel lean condition, the distance between peaks varied little between the midflame and the far-flame profile. At an equivalence ratio of 0.55, the 4:1 AR elliptical burner flame was very short thus there was not much time for the jet to diverge.

Of note was that the cold jet near-burner equivalence ratio of 0.55 profile showed very strong splitting, but this splitting in velocity was not seen in the flame result. Most likely, this was not due to lack of splitting in the velocity field, but lack of adequate seeding at the edges of the 4:1 AR elliptical burner flame. For all cases, flame or cold jet, there was a significant axial velocity at the centerline compared to the maximum velocity which occurred at the split jets.

The normalized RMS of the velocity of the 4:1 AR elliptical burner laminar flame was greater for the cold jet for all cases. The 4:1 AR elliptical burner flame RMS of the velocity had a strong double peak structure for the near-burner and midflame regions for an equivalence ratio of 0.55 and at the near-burner for an equivalence ratio of 1.0. The peaks in the normalized RMS of the velocity appeared to line up with slight depressions seen in the velocity profile. There was a slight double peak structure seen for the far-

flame profile for an equivalence ratio of 0.55, the midflame and far-flame profiles for an equivalence ratio of 1.0, and the midflame profile of equivalence ratio of 2.0 where the profile of the RMS of the velocity mirrored the velocity profile in shape. For an equivalence ratio of 2.0 at the near-burner and for an equivalence ratio of 4.0 at the near-burner and midflame profiles, the RMS of the velocity increased in regions of large velocity change, i.e., on both sides of the velocity peak. All other cases showed the RMS of the velocity being constant across the detection region.

While comparing the 3:1 AR elliptical burner with the 4:1 AR elliptical burner, it was noticed that the 3:1 AR elliptical burner for all laminar flame conditions had a higher maximum gas velocity. Similarly, for the cold jet, the 3:1 AR elliptical burner continued to have higher maximum axial velocity for a given axial location except in the near-burner of equivalence ratio of 0.55 jet, where the 4:1 AR elliptical burner had a larger maximum jet velocity.

The 3:1 AR elliptical burner produced a higher flame RMS of the velocity than the 4:1 AR elliptical burner for all cases except at the midflame for an equivalence ratio of 0.55 and at the far-flame profiles of equivalence ratios of 1.0 and 2.0. At these exceptions, the RMS of the velocity was similar between the burners. For the cold jet, the 3:1 AR elliptical burner maximum RMS of the velocity was similar to that of the 4:1 AR elliptical burner for many cases. The 3:1 AR elliptical burner had a lower cold jet normalized RMS of the velocity than the 4:1 AR elliptical burner at an equivalence ratio of 0.55 at the midflame. At an equivalence ratio of 1.0 far-flame with a cold jet and the near-burner of equivalence ratio of 4.0 with the cold jet, the 4:1 AR elliptical burner.

## 5.1.2 Schlieren Imagery:

**5.1.2.1 General Observations:** Due to a lack of observable structure in the flame downstream of the premixed flame zone, only near-burner schlieren results are presented (Figs. 5.1.6 to 5.1.8).

An inner premixed cone structure was easily observed and was sharply defined for the lean to stoichiometric fuel/air mixtures. With the rich flames, however, the inner premixed cone structure was less distinct. This corresponds to what was seen with the visual images. As premixing was reduced (increasing the equivalence ratio), a lesser proportion of the total energy release (and change from a fuel/air to product mixture) occurred at the premix boundary of the flame. This would lead to the reduction in the strength of gradients of the flame.

Larger gradients were seen across the inner cone boundary than across the outside diffusion flame for all conditions. Premixed reactions are, in general, faster than diffusion reactions due to reduction on the need for slow mixing processes, thus they should have a thinner reaction zone (with a corresponding increase in gradient).

**5.1.2.2 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** For equivalence ratios of 0.55 and 1.0 (Figs. 5.1.6 and 5.1.7), the circular burner produced inner premixed cones that were slightly longer than that of the 3:1 AR elliptical burner. The 3:1 AR elliptical burner, for a given height above the burner exit, had a wider major axis inner cone and narrower major axis outer flame region than the circular burner. For the minor axis schlieren images, there was a narrower inner cone with wider outer flame

than the circular burner. This indicates that the outer flame region grew faster for the minor axis than the major axis.

Visually, the gradients of the inner cone were weaker for the major axis than the minor axis, while the relative intensity of the outer flame gradients appeared somewhat similar between the major and minor axis with the minor axis having a slightly more gradual gradient. For a given gradient a longer path will produce a greater deflection. Thus the minor axis images will have a more intense gradient due to the increased path length.

The inner cone of the circular burner came to a sharp point at an equivalence ratio of 0.55, while the 3:1 flame inner cone converged to an indistinct (from the major axis view) edge parallel to the major axis of the burner. From the minor axis view, the 3:1 AR elliptical burner schlieren images show a sharp point. The 3:1 AR elliptical burners inner cone also seemed to exhibit a small amount of bifurcation (implied from a gradient located at the centerline of the jet) similar to what was observed in the flame images at an equivalence ratio of 0.55. Both the circular and 3:1 AR elliptical burner flames exhibited sharp inner cone points at an equivalence ratio of 1.0, but the 3:1 AR elliptical burner point was somewhat indistinct in the major axis image.

With the rich flames of equivalence ratios of 2.0 and 4.0, the 3:1 AR elliptical burner inner cone was still wider on the major axis and narrower on the minor axis than the circular burner inner cone, however, the outer flame zone on the major axis appeared to have a similar width to the circular burner with the minor axis being slightly wider than the circular outer flame. The core of the inner flame appeared to have an internal gradient. There was no apparent axis switching of the inner cone for any condition tested. The axis switching seen in the flame images and velocity profile widths was apparently decoupled from the density gradients of the flame.

5.1.2.3 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners: For all equivalence ratio flames, the 4:1 AR elliptical burner inner cone was much shorter than the 3:1 AR elliptical burner as was seen in the flame images. The 4:1 AR elliptical burner inner cone appeared to split into two jets immediately upon leaving the burner. The outer flame cone also consisted of two flame regions given the presence of a centerline gradient. The two inner cone jets in the major axis narrowed very quickly while in the minor axis plane, the inner cone jets increased in width. The 4:1 AR elliptical burner seemed to have a much stronger gradient in the outer flame outside edge (particularly in the minor axis view). For equivalence ratios of 1.0 and greater, the gradients seen at the tips of the two inner cone jets were very faint in the images of the minor axis compared to the strong gradients apparent at the tips in images of the major axis. As the equivalence ratio increased the gradient between the two diffusion type flames became increasingly faint indicating a coalescence of the two outer flames. Increasing the equivalence ratio also tended to show increased asymmetry between the two inner cone jets emitted from the burner.

#### 5.2: Temperature Studies

**5.2.1 General Observations:** The traverse temperature distribution of the laminar flames (20 m/s) of the three burners at three flame profile heights (12.5%, 25%, and 50% of flame length) and four equivalence ratios (0.55, 1.0, 2.0, and 4.0) are shown in Figs 5.2.2a to 5.2.5c. The turbulent flame (100 m/s) profiles are given in Figs. 5.2.6a to c.

Hariharan (2004) did a study of the flame properties of a similar propane/hydrogen mixture, but his flames had a burner exit velocity of 40 m/s and had an induced turbulence while the current study is laminar with a jet exit velocity of 20 m/s. The peak flame temperatures of this study match reasonably well with those found by Hariharan (Table 5.2) despite these differences.

**5.2.2 Effect of Level of Premixing:** Figures 5.2.1a to c show the effect of equivalence ratio on the peak flame temperature for the three profile heights of the flames. In general, for the burners, increasing the equivalence ratio from 0.55 to 1.0 caused the peak flame temperature to increase. As the equivalence ratio increased from stoichiometric to rich conditions the peak temperature decreased slightly for the burners. Lean flames have an excess of oxygen and nitrogen that will act as a diluent and heat sink to the flame, thus producing a lower temperature (compared to a stoichiometric fuel/air mixture). In the fuel rich flames, there was decreasing amounts of premixed air in the unburned fuel/air jet, thus the flames became more dependent on mixing with the surrounding air. This slows the reaction rate of the flame, lowering the temperature.

Increasing the equivalence ratio had the following effects on the temperature profiles (Figs. 5.2.2a to c, 5.2.3a to c, 5.2.4 a to c, and 5.2.5a to c). First, the temperature

profiles tended to get narrower with increased equivalence ratio for all burners and profile heights. This was contrary to what was seen with the velocity profiles. In addition, a cooler core region of the flame, corresponding to a core of unburned fuel, tended to exist at a greater axial distance of the flame with increase in equivalence ratio. Increasing the equivalence ratio to greater than stoichiometric will lead to reduce the flame velocity; thus the flame will establish farther away both in radial distance from the centerline and axial distance from the burner.

**5.2.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** For lean to stoichiometric equivalence ratios, the circular burner produced a higher peak flame temperature than the 3:1 AR elliptical burner at the near-burner. The magnitude of the peak temperature was similar between the 3:1 AR elliptical burner and the circular burner at the midflame and far-flame.

Rich (equivalence ratio of 2.0 and 4.0) flames established with the 3:1 AR elliptical burner produced higher peak flame temperatures at the midflame and far-flame locations when compared to the circular burner. At the near-burner, the peak flame temperature of the two burners was similar. The enhanced mixing provided by the elliptical burner allowed more air to be present in the flame zone of with the 3:1 AR elliptical burner. This allowed the rich flames of the 3:1 AR elliptical burner to extract more energy from the fuel over a shorter distance, thus producing a higher flame temperature. The enhanced mixing would be more prevalent at greater distances from the burner; this results in the similarity of the flame temperatures at the near-burner.

While comparing temperature profiles, a double peak structure was seen at the near-burner for all equivalence ratios for both the circular burner and 3:1 AR elliptical burner. A 'double peak' structure was where there was a cooler inner region of the combusting jet that was surrounded by two peaks in temperature. This cooler inner region consisted of unburned reactants. At the midflame height, the 3:1 AR elliptical burner showed a double peak for equivalence ratios of 0.55 and 4.0, while the circular burner showed a double peak at equivalence ratios of 2.0 and 4.0. The peaks for the 3:1 AR elliptical burner on the major axis were a greater distance apart than the double peaks exhibited by the circular burner. No double peaks were seen at the far-flame.

In addition, both the 3:1 AR elliptical burner and the circular burner exhibited regions of constant flame temperature. For the near-burner, these temperature plateaus were seen for equivalence ratios of 1.0 and 2.0 for the 3:1 AR elliptical burner (ranging from an  $r/d_{eff}$  of 0.6 to 1.0 for both equivalence ratios) and for equivalence ratios of 2.0 (ranging from 0.3 to 0.6  $r/d_{eff}$ ) and 4.0 (ranging from 0.4 to 0.6  $r/d_{eff}$ ) for the circular burner.

At the midflame, both the circular burner and the 3:1 AR elliptical burner had regions of small temperature variation with increase in radial distance. For an equivalence ratio of 1.0, this occurred from the centerline to a  $r/d_{eff}$  of 0.5 for the circular burner and from the centerline to a  $r/d_{eff}$  of 0.6 for the 3:1 AR elliptical burner. This region was from a  $r/d_{eff}$  of 0.3 to 0.7 for an equivalence ratio of 2.0 with flames produced by the circular burner and from the centerline to a  $r/d_{eff}$  of 1.0 for the 3:1 AR elliptical burner. At an equivalence ratio of 4.0 a constant temperature was seen from a  $r/d_{eff}$  of 0.8 to 1.4 for the 3:1 AR elliptical burner. The circular

burner also had a plateau for an equivalence ratio of 0.55 (ranging from the centerline to a  $r/d_{eff}$  of 0.3 at the midflame; the behavior was not seen in the 3:1 AR elliptical burner at that flame height.

A temperature plateau was seen with all far-flame conditions for the 3:1 AR elliptical burner, although for equivalence ratios of 0.55 and 4.0 there was a slight decrease in temperature from a peak at the centerline with increase in radial location across the 'constant' temperature region. These regions of constant temperature ranged from the centerline to a  $r/d_{eff}$  of 1.4 for an equivalence ratio of 0.55, to a  $r/d_{eff}$  of 0.6 for an equivalence ratio of 1.0, and to a  $r/d_{eff}$  of 1.2 for equivalence ratios of 2.0 and 4.0. At the far-flame, the circular burner's region of 'constant' temperature ranged from the centerline to a  $r/d_{eff}$  of about 0.5 to 0.6 for all equivalence ratios.

The 3:1 AR elliptical burner temperature profiles were wider than the circular burner profiles when comparing the distance between the double peaks of temperature, the width of any constant temperature zones, and the location where the temperature reached atmospheric conditions at all flame conditions and heights. At regions of decrease in temperature with increase of radial distance (i. e., the edge of the flame), for the lower equivalence ratios of 0.55 and 1.0, the 3:1 AR elliptical burner tended to have a lower rate of temperature decline compared to the circular burner, particularly in the midflame profiles. With the rich flames, the rate of temperature decrease was similar for the 3:1 AR elliptical burner and circular burner.

At the near-burner, the widths of the major and minor radial temperature profiles were similar. However, at the midflame and higher, the minor axis temperature profile was wider than that of the major axis. This axis switching is consistent with the velocity profile widths seen earlier.

**5.2.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:** While comparing peak flame temperatures, it was seen that the flame temperature for the 4:1 AR elliptical burner was lower than that of the 3:1 AR elliptical burner at the near-burner for an equivalence ratio of 2.0, and at the midflame for equivalence ratios of 0.55 and 2.0. The 4:1 AR elliptical burner also produced a lower peak flame temperature than the 3:1 AR elliptical burner at the far-flame for an equivalence ratio of 4.0. The 4:1 AR elliptical burner at the far-flame for an equivalence ratio of 4.0. The 4:1 AR elliptical burner produced a greater peak temperature at the near-burner for an equivalence ratio of 0.55 and at the far-flame of equivalence ratio of 1.0. All other conditions and profiles produced similar peak temperatures between the 4:1 AR elliptical and 3:1 AR elliptical burners.

The dual jet structure seen for the 4:1 AR elliptical burner with the flame images and velocity profiles was again evident in the temperature profiles. This was seen most prominently through a quadruple peak structure observed in the temperature profile at the midflame for an equivalence ratio of 2.0. A 'quadruple peak' structure was given by four temperature peaks in the profile. This indicated that there were two flame zones bracketing two cooler unreacted fuel/air mixture jets leaving the burner. The centerline region of reduced temperature consisted of post combustion gases cooled by interaction with the quiescent air.

A constant temperature plateau structure (similar to what was seen with the circular and 3:1 AR elliptical burners) was evident for the 4:1 AR elliptical burner at the

midflame for the flames of equivalence ratio of 1.0 and 2.0. At the far-flame, the temperature profiles had wide regions of semi-constant temperature, with a tendency for the temperature to slightly decrease with increasing radial position. The far-flame temperature profile exhibited a cooler centerline with two regions of high temperature symmetric to the centerline at equivalence ratio of 1.0. All other cases showed a wide centerline to edge of flame region of very little temperature variation. This constant temperature region increased in width with increase in equivalence ratio.

In all cases, the 4:1 AR elliptical burner produced wider flames than the 3:1 AR elliptical burner with the greatest differences occurring at higher equivalence ratio. Increased equivalence ratio leads to an increase in flame length which caused the peaks of the 4:1 AR elliptical burner flame to be farther apart due to the jet splitting angle.

**5.2.5 Turbulence Effects on Burners:** The turbulent flames (Fig. 5.2.6.a to c) exhibited slightly (~150K) lower peak flame temperatures than the laminar flames of this study. This was likely due to the additional mixing provided by turbulence diluting the flame thus reducing the flame temperature. These turbulent flame temperatures match what was seen by Hariharan (2004).

The turbulent 4:1 AR elliptical burner had a lower peak temperature than the other two burners, particularly at the near burner region. This indicates that the 4:1 AR elliptical burner had increased mixing with the ambient air, compared to the other burners which reduced the temperature through dilution.

#### 5.3: In-flame Species Concentration Profiles

**5.3.1 General Observations:** At an equivalence ratio of 4.0, the peak values of the NO concentration for the mid and far-flame profiles for the 4:1 AR elliptical burner were unreasonably higher with the peak NO concentration unexpectedly being 2 to 2.5 times greater than the highest NO concentration for the 3:1 AR elliptical burner. Due to the relatively large width of the rich 4:1 AR elliptical burner flame, it was likely that some heating of the probe occurred distorting the NO results for the 4:1 AR elliptical burner. This inflation tended to be greater at the central regions of the flame, thus, artificially inflating the results. Therefore, due to the uncertainty in the correctness of these results, the midflame and far-flame profiles of the NO concentration at a velocity of 20 m/s and equivalence ratio of 4.0 will not be presented here.

Comparing the current results to previous studies is difficult given the lack of work with 40% hydrogen by mass in propane flames. Table 5.3 summarizes one similar study.

The peak concentrations of the laminar flames of this study do not match very well the results of Hariharan (2004) For a circular burner at similar flame height percentages, with an equivalence ratio of 1.0, Hariharan obtained a much lower peak CO concentration and a similar NO and  $CO_2$  concentration to the laminar flames of the current study. With flames of equivalence ratio of 4.0, Hariharan measured a much lower peak CO concentration, a higher peak  $CO_2$  concentration, and a much higher peak NO concentration. The differences between the values are likely due to the turbulence effects. As was mentioned in Section 5.2.1, the flames of the Hariharan study had an induced turbulence. A turbulent flame is likely to have much less CO than a laminar

flame due to enhanced mixing with outside air diluting concentrations or increasing the local combustion efficiency. The comparison of the turbulent flame of this study with Hariharan (2004) shows a much better match for the CO and  $CO_2$  peak concentrations.

### **5.3.2 Effect of Level of Premixing:**

**5.3.2.1 Carbon Monoxide:** With an increase in equivalence ratio there was a decrease in the peak CO concentration at the near-burner profiles for the circular burner (Figs. 5.3.1a-c). For the 3:1 AR elliptical burner at the near-burner, the peak CO concentration increased with increase in equivalence ratio of 0.55 to 1.0, then decreased with change of equivalence ratio from 1.0 to 4.0. The 4:1 AR elliptical burner near-burner profile had a decrease in the peak CO concentration with increase of equivalence ratio of 0.55 to 2.0 but the peak CO concentration increased with increase in equivalence ratio of 0.55 to 2.0 but the peak CO concentration increased with increase in equivalence ratio of 0.55 to 2.0 but the peak CO concentration increased with increase in equivalence ratio from an equivalence ratio of 2.0 to 4.0.

At the midflame, the circular burner had an increase in the peak measured CO concentration with an increase in equivalence ratio from 0.55 to 1.0 then decreased from an equivalence ratio of 1.0 to 4.0. For the 3:1 AR elliptical burner at the midflame, the peak CO concentration increased with increase of equivalence ratio from 0.55 to 1.0 and then slightly decreased in peak CO concentration from an equivalence ratio of 1.0 to 4.0. The 4:1 AR elliptical burner peak CO concentration increased from an equivalence ratio of 1.0 to 4.0 for the midflame ratio of 1.0 to 2.0, and increased from an equivalence ratio of 2.0 to 4.0 for the midflame profile.

With equivalence ratios of 1.0 to 4.0, at the far-flame, all three burners had an increase in peak CO concentration with increase in equivalence ratio. An increase of

equivalence ratio of 0.55 to 1.0 caused an increase in peak CO concentration for the circular burner, the 3:1 AR elliptical burner CO concentration remained constant, and the 4:1 AR elliptical burner had a decrease in peak CO concentration.

The location of the axial peak CO concentration for the burners tended to move downstream as the equivalence ratio was increased. Flames with an equivalence ratio of 0.55 had the peak located at the near-burner, at an equivalence ratio of 1.0 the CO concentration peaked at the midflame, the equivalence ratio of 2.0 flame had a peak located between the midflame and far-flame profiles, and for an equivalence ratio of 4.0 the CO concentration peak was found at the far-flame (or higher).

With increased equivalence ratio, there should be a decrease in the combustion efficiency (due to the necessity for additional mixing with the ambient air). The reduction of oxygen availability with the increase in equivalence ratio will lead to an increase in incomplete combustion products, such as CO, particularly at the near-burner region. This would be indicated by an increase in CO concentration at a particular height of a flame. There will also be a tendency for the bulk of the combustion to shift to a greater height above the burner with an increase in equivalence ratio. This is due to a reduction in the flame velocity as the flame became more fuel rich resulting in the need to entrain additional air to complete combustion. This will tend to delay the axial development of the reaction zone of the flame.

**5.3.2.2 Carbon Dioxide:** At the near-burner (Fig. 5.3.1d), increasing the equivalence ratio decreased the peak  $CO_2$  concentration for the range of equivalence ratios of 0.55 to 4.0 for the circular burner. For the 3:1 AR elliptical burner, the peak  $CO_2$ 

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concentration decreased with the increase in equivalence ratio over the range of equivalence ratios of 1.0 to 4.0. The range of equivalence ratios of 0.55 to 2.0 produced a constant peak  $CO_2$  concentration for the 4:1 AR elliptical burner. There was an increase in the peak  $CO_2$  concentration for increase in the equivalence ratio from 0.55 to 1.0 for the 3:1 AR elliptical burner and for the 4:1 AR elliptical burner from an equivalence ratio of 2.0 to 4.0.

At the midflame (Fig. 5.3.1e), the circular burner flame peak  $CO_2$  concentration decreased with increasing equivalence ratio for equivalence ratios from 1.0 to 4.0. The 3:1 AR elliptical burner showed a decrease of the peak  $CO_2$  concentration with equivalence ratio from 1.0 to 2.0 but it remained constant from equivalence ratios of 2.0 to 4.0. In the 4:1 AR elliptical burner the peak  $CO_2$  concentration was constant from equivalence ratios of 0.55 to 2.0 then increased with further increase in equivalence ratio to 4.0. For a change of equivalence ratio from 0.55 to 1.0, the circular and 3:1 AR elliptical burners had an increase in the peak  $CO_2$  concentration.

At the far-flame (Fig. 5.3.1f), there was a decrease in the peak CO<sub>2</sub> concentration for the circular burner with the change in equivalence ratio of 0.55 to 1.0, an increase from an equivalence ratio of 1.0 to 2.0, and a decrease from an equivalence ratio of 2.0 to 4.0. The 3:1 AR elliptical and 4:1 AR elliptical burners increased their peak CO<sub>2</sub> concentration with the increase in equivalence ratio from 0.55 to 1.0. The 3:1 AR elliptical burner flame slightly increased its peak CO<sub>2</sub> concentration with increase in equivalence ratio of 1.0 to 2.0 while, for the 4:1 AR elliptical burner, it slightly decreased for this change. The 3:1 AR elliptical burner decreased in peak CO<sub>2</sub> concentration from an equivalence ratio of 2.0 to 4.0 while the 4:1 AR elliptical burner exhibited an increase in peak  $CO_2$  concentration.

In general, for the three burners, there was a widening of the  $CO_2$  concentration profiles with an increase in equivalence ratio and the peak concentration of  $CO_2$  was highest at the far-flame region. For rich mixtures, the fuel must mix with the quiescent air; this results in the widening of the flame. The CO to  $CO_2$  reaction is rather slow, thus it would be expected that  $CO_2$  concentration would increase with height of the flame.

**5.3.2.3** Nitric Oxide: An increase in the equivalence ratio caused an increase in the peak NO concentration for all profiles for the 4:1 AR elliptical burner (Fig. 5.3.1g to i). There was an increase in the peak NO concentration for the circular burner with increasing equivalence ratio except at the near-burner for the range of equivalence ratios of 2.0 to 4.0 (where the peak NO concentration dropped), and for the range of equivalence ratios of 0.55 to 2.0 at the midflame where the peak NO concentration was similar. For the 3:1 AR elliptical burner, there was an increase of peak NO concentration with increase in equivalence ratio in all profiles except in the far-flame region from equivalence ratios of 2.0 to 4.0 where there was a decrease.

An increase in the peak NO concentration with increase in equivalence ratio was expected due to the increase of the length of the flame thereby increasing the residence time. The decrease from an equivalence ratio of 2.0 to 4.0 seen for the circular and 4:1 AR elliptical burner corresponded to the reduction in temperature seen previously. At an equivalence ratio of 4.0, the flame was mixing limited thus a lower flame temperature was produced, reducing the peak NO production.

**5.3.2.4 Oxygen:** The centerline oxygen level was reduced with an increase in equivalence ratio for all burners. Increasing the equivalence ratio resulted in a decrease in the proportion of air in the premixed mixture, so the oxygen concentration was reduced. The lack of  $O_2$  concentration at the far-flame for a lean equivalence ratio of 0.55 (where it would be expected that some  $O_2$  would be present) indicates that much of the atomic oxygen must be in CO, O, OH or other oxygenated compounds rather than in  $O_2$ .

### 5.3.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:

**5.3.3.1 Carbon Monoxide:** The 3:1 AR elliptical burner produced a significantly lower peak CO concentration (Fig 5.3.1.a to c) than the circular burner at the near-burner and midflame profile heights for an equivalence ratio of 0.55 and at the midflame for an equivalence ratio of 1.0. Higher peak CO concentrations were produced by the 3:1 AR elliptical burner for an equivalence ratio of 4.0 at the near-burner and midflame heights and in the far-flame for equivalence ratios of 0.55 and 2.0

Figures 5.3.2a to c, 5.3.3a to c, 5.3.4a to c, and 5.3.5a to c give the radial profiles of CO concentration for the burners. Both the circular and 3:1 AR elliptical burners exhibited the 'double peak' structure characteristic of a flame front bounding an uncombusted jet for all equivalence ratios at the near-burner and at the midflame for the rich conditions of equivalence ratios of 2.0 and 4.0. In addition, the 3:1 burner also exhibited a 'double peak' at an equivalence ratio of 0.55. In general, the double peaks of the circular burner and the 3:1 AR elliptical burner major axis profile occurred at similar radial locations. However, at the near-burner of the equivalence ratio of 0.55, the 3:1 AR

elliptical burner CO concentration major axis profile was slightly wider than that of the circular burner. Also, the circular burner produced wider CO concentration profiles at an equivalence ratio of 2.0 at the near-burner, for equivalence ratios of 0.55 and 1.0 at the midflame profile, and in the far-flame for equivalence ratio of 1.0

Comparing the minor to major axis of the 3:1 AR elliptical burner (Figs. 5.3.3ac), the minor axis produced a reduced peak CO concentration and had a narrower profile width than the major axis at the near-burner region for equivalence ratios of 1.0 and 4.0. At the midflame region, for an equivalence ratio of 1.0, the 3:1 AR elliptical burner produced similar minor and major axis peak concentrations and profile widths. For an equivalence ratio of 4.0, the midflame minor axis profile showed a similar width as the midflame major axis profile but had a reduced CO concentration. At the far-flame, for an equivalence ratio of 1.0 the flame had similar peak concentrations between the major and minor axis profiles but a wider minor axis profile. At an equivalence ratio of 4.0, the flame had similar peak concentrations and width between the major and minor axis.

**5.3.3.2 Carbon Dioxide:** The circular burner produced a greater peak  $CO_2$  concentration (Figs. 5.3.1d to f) for all profile heights for an equivalence ratio of 0.55, at the near-burner and midflame heights for an equivalence ratio of 1.0 and at the far-flame for an equivalence ratio of 2.0. Greater  $CO_2$  concentrations were measured for the 3:1 AR elliptical burner for all flame heights at an equivalence ratio of 4.0. This corresponds to the increased flame temperature seen for the 3:1 AR elliptical burner at these conditions. Both increased flame temperature and increased  $CO_2$  concentration are indicative of more complete combustion.

The circular and 3:1 AR elliptical burners exhibited a 'double peak' structure in the CO<sub>2</sub> concentration profiles for all near-burner and midflame cases (Figs. 5.3.2d to f, 5.3.3d to f, 5.3.4d to f, and 5.3.5d to f). At the far-flame, a 'double peak' was seen for both the circular and the 3:1 AR elliptical burner for an equivalence ratio of 4.0, and for the 3:1 AR elliptical burner only for an equivalence ratio of 2.0. A significant centerline concentration of CO<sub>2</sub> was seen for all far-flame cases with 'double peaks' for both burners and the equivalence ratio of 0.55 circular burner midflame profile. The circular and 3:1 AR elliptical burner 'double peaks' occurred at similar radial positions at the near-burner and at the midflame for rich equivalence ratios. For the lean to stoichiometric profiles at the midflame, the circular burner had a wider CO<sub>2</sub> profile than the 3:1 AR elliptical burner.

The major axis produced greater peak  $CO_2$  than the minor axis (Figs. 5.3.3d to f and 5.3.5d to f) at the near-burner and midflame regions for an equivalence ratio of 1.0. The major axis profile was slightly wider than the minor axis profile at the near-burner and midflame regions, although the radial location of the 'double peaks' were roughly the same. At the far-flame, the major and minor axis profiles both peaked at the centerline with the minor axis profile being wider than the major axis profile, an apparent axis switching.

For an equivalence ratio of 4.0, the near-burner peaks were similar in magnitude with the major axis  $CO_2$  concentration profile being wider, the midflame had a greater  $CO_2$  concentration on the major axis with the major axis being wider, and the far-flame produced a greater concentration on the minor axis with a wider profile, again, another evidence of axis switching.
**5.3.3.3 Nitric Oxide:** The circular burner had a greater peak NO concentration (Fig. 5.3.1g to i) at all flame heights for an equivalence ratio of 0.55 and at the nearburner and far-flame regions for an equivalence ratio of 2.0. The 3:1 AR elliptical burner had a greater peak NO at all flame heights for the flame of equivalence ratio of 4.0, and at the midflame and far-flame profiles for an equivalence ratio of 1.0.

A 'double peak' structure was seen for all profiles (Figs. 5.3.2g to i, 5.3.3g to i, 5.3.4g to i, and 5.3.5g to i) except at the far-flame region for an equivalence ratio of 2.0 for both the circular and the 3:1 AR elliptical burners.

The minor axis of the flames of equivalence ratio of 1.0 and 4.0 produced a greater NO peak than that of the major axis in all flame regions.

**5.3.3.4 Oxygen:** A central core of oxygen was seen for both the circular and 3:1 AR elliptical burners profiles (Figs. 5.3.2j to l, 5.3.3j to l, 5.3.4j to l, and 5.3.5j to l) at the near-burner for all equivalence ratios, and at the midflame for equivalence ratios of 2.0 and 4.0 with both burners. In addition a narrow oxygen core was seen at the midflame equivalence ratio of 0.55 for the 3:1 AR elliptical burner. In general, at the near burner, the peak oxygen concentration at the centerline was similar between the two burners, but for the near-burner region for an equivalence ratio of 0.55, the 3:1 AR elliptical burner that a greater peak  $O_2$  concentration than the circular burner. This increased peak at the near-burner region likely led to the presence of oxygen at the core of the flame at the midflame for the equivalence ratio of 0.55 mentioned previously.

The 3:1 AR elliptical burner had a wider near-burner central oxygen core on the major axis than the circular burner with the 3:1 AR elliptical minor axis being narrower than that of the circular. At the midflame (where the oxygen core only existed for rich flames) the central oxygen cores had similar maximum values and shapes between the burners. The circular burner had wider overall  $O_2$  deficit regions defined as the width of the region with very low oxygen levels corresponding to the flame zone/reaction products. Lower equivalence ratios tended to have greater differences in the  $O_2$  deficit region width while comparing the 3:1 AR elliptical and circular burners.

# 5.3.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Aspect Ratio Elliptical Burners:

**5.3.4.1 Carbon Monoxide:** There was only one condition, at the near-burner for an equivalence ratio of 0.55, that the 4:1 AR elliptical burner produced a higher peak CO concentration than the 3:1 AR elliptical burner. The 3:1 AR elliptical burner had a greater peak CO concentration than the 4:1 AR elliptical burner at the near-burner for equivalence ratios of 1.0 and 2.0, the midflame of equivalence ratio of 0.55 to 2.0, and for the far-flame from equivalence ratios of 1.0 to 4.0. The other profiles and equivalence ratios showed similar peak CO concentrations.

The splitting characteristics of the 4:1 AR elliptical burner seen in previous sections was also apparent in the CO profiles (Figures 5.3.2a to c, 5.3.3a to c, 5.3.4a to c, and 5.3.5a to c). A 'triple peak' structure (a significant centerline concentration of CO with two other peaks bracketing two regions of lower CO concentration) could be seen in all near-burner profiles. For low equivalence ratios, the peaks bracketing the centerline

were of lower concentration compared to the central peak, but with increasing equivalence ratio the magnitude of the bracketing peaks increased to a similar level as the central peak. At the midflame, the 4:1 AR elliptical burner CO concentration profiles were characterized by having a non-zero centerline value which then increased with increased radial position to a peak. This peak then decreased to a non-zero minimum then increased to another CO peak with further increases in radial distance. After this second peak, the CO concentration decreased to atmospheric values. Since each of the CO peaks corresponded to a flame front, there was an unburned fuel/air core still existing at the midflame. This was confirmed by an increase in the local oxygen concentration at the same radial location as the CO profile dip, as will be shown later. At the far-flame, the CO concentration increased slowly with increasing radial position to a peak far from the centerline. This peak value then decreased quickly to atmospheric values. For the rich flames of equivalence ratios of 2.0 and 4.0, a multiple peak structure could still be faintly discerned, but the peak on the centerline side was of a much reduced magnitude compared to the outside peak. Compared to the 3:1 AR elliptical burner, the 4:1 AR elliptical burner produced much wider CO concentration profiles with a much more complicated structure.

**5.3.4.2 Carbon Dioxide:** The 4:1 AR elliptical burner had a lower peak  $CO_2$  concentration compared to the 3:1 AR elliptical burner for equivalence ratios of 1.0 and 2.0 at the near-burner, the range of equivalence ratios of 0.55 to 2.0 at the midflame, and at all far-flame profiles. The 4:1 AR elliptical burner produced higher  $CO_2$  concentration only at the near-burner for an equivalence ratio of 4.0.

The CO<sub>2</sub> profiles, similar to the CO distributions, showed a 'triple peak' structure at all near-burner and midflame profiles. Regions of constant CO<sub>2</sub> concentration were seen at the near-burner equivalence ratios of 1.0 and 2.0, at the midflame for equivalence ratios of 0.55 to 2.0, and at the far-flame for all equivalence ratios.

**5.3.4.3 Nitric Oxide:** At the near-burner, the peak NO concentrations for the 4:1 AR elliptical burner were much smaller than that of the 3:1 AR elliptical burner particularly at equivalence ratios of 0.55 and 1.0 where the NO concentration was negligible for the 4:1 AR elliptical burner. For an equivalence ratio of 0.55, the 4:1 AR elliptical burner had a peak NO concentration similar to that of the 3:1 AR elliptical burner at all profile heights. At an equivalence ratio of 1.0, the 3:1 AR elliptical burner produced greater peak NO concentration at both the midflame and far-flame profiles. At the midflame and far-flame for equivalence ratios of 2.0, the 4:1 AR elliptical burner produced a greater peak NO concentration than the 3:1 AR elliptical burner. Structurally, the 4:1 AR elliptical burner produced multiple peaks in the radial NO concentration profile similar to what was seen with the CO and CO<sub>2</sub> profiles. Peaks were not seen for the near-burner equivalence ratio of 0.55 and 1.0 flames (due to the presence of only negligible NO) and for the equivalence ratios of 1.0 and 2.0 for the far-flame, which had constant central regions of NO.

**5.3.4.4 Oxygen:** The multiple peak structure seen in the previous emissions profiles for the 4:1 AR elliptical burner was less obvious with the oxygen profiles. Multiple peaks of  $O_2$  concentration were seen for all near-burner cases, but the outside

flame edge for equivalence ratios of 1.0 and 2.0 had a very narrow outside jet oxygen deficit region. For an equivalence ratio of 0.55 the outside edge flame region maintained a relatively high  $O_2$  content. This multiple peak structure continued into the midflame region for all equivalence ratios but 1.0. At the far-flame, a central core region of oxygen appeared for equivalence ratios of 1.0, 2.0 and 4.0, likely due to the splitting of the flame allowing air to occupy in between the jets.

## 5.3.5 Turbulence Effects on Burners:

**5.3.5.1 Carbon Monoxide:** For a given height above the burner for all three burners, the turbulent flame (Fig. 5.3.6 a to c) produced a lower peak CO concentration than the laminar flames, particularly at the mid-flame and far-flame regions. Similar to what was seen with the laminar flame, the 4:1 AR elliptical burner produced a higher peak CO concentration than the circular and 3:1 AR elliptical burners at the near-burner and midflame regions and a lower peak CO concentration at the far-flame, with the difference being greater at the midflame. The 3:1 AR elliptical and circular burners produced similar peak CO concentrations for the near-burner and far-flame regions. At the midflame, the circular burner produced a slightly lower peak CO concentration than the 3:1 AR elliptical burner. A turbulent flame will entrain much more of the ambient air than a laminar flame. This increases the availability of oxygen which will increase the rate of the consumption of CO in the flame.

The width of the CO concentration profiles of the turbulent flame were similar to the widths of the laminar flame at the near-burner and midflame regions for all three burners. At the far flame, the turbulent flame had a greater CO concentration profile width for the 3:1 AR elliptical and circular burners. For the 4:1 AR elliptical burner, the distance between the peaks in the CO concentration profiles was similar between the laminar and turbulent flames at the far-flame, but the turbulent flame decreased to ambient values at a much reduced rate compared to the laminar flame.

For the turbulent flame, the widths of the CO concentration profiles were similar between the circular and 3:1 AR elliptical burner while the 4:1 AR elliptical burner CO concentration profiles were much wider than the other two burners. It would appear that the freezing of the reactions seen for the laminar 4:1 AR elliptical burner also holds for the turbulent flame. This is supported by the lower temperatures combined with the increased CO concentration seen for the turbulent 4:1 AR elliptical burner compared to the other two burners.

The major and minor axis profiles of the 3:1 AR elliptical burner produced similar peak CO concentrations. At the near-burner profile, the major axis CO concentration profile was wider than the minor axis, but for the midflame and far-flame regions, the CO concentration profile widths were similar. No axis switching was apparent from the CO concentration profiles for the turbulent 3:1 AR elliptical burner flame.

**5.3.5.2 Carbon Dioxide:** The turbulent flames (Fig. 5.3.6d to f) produced much greater peak  $CO_2$  concentrations when compared to the laminar flames for the nearburner and midflame regions of the 3:1 AR elliptical and circular burners. At the farflame, the peak  $CO_2$  concentration was similar between the laminar and turbulent flames for the 3:1 AR elliptical and circular burners. The 4:1 AR elliptical burner produced similar peak  $CO_2$  concentrations between the turbulent and laminar flames at the nearburner and midflame profiles, and a reduced peak  $CO_2$  concentration at the far-flame. As was mentioned in Section 5.3.5.1, the CO consumption was increased in the turbulent flame due to increased oxygen availability. This will lead to increased  $CO_2$  concentration since the CO is converted to  $CO_2$ .

The width of the  $CO_2$  concentration profiles was narrower at the near-burner and midflame profiles for the circular and 3:1 AR elliptical turbulent flames, but the turbulent flame was wider at the far-flame profile. The 4:1 AR elliptical burner  $CO_2$  concentrations were wider for the turbulent flame for all flame regions.

The 3:1 AR elliptical burner and the circular burner produced similar peak  $CO_2$  concentrations with similar widths for the three flame heights. The 3:1 AR elliptical and circular burners produced much greater peak  $CO_2$  concentrations than the 4:1 AR elliptical burner for all flame regions, but the difference was particularly great at the nearburner and midflame profiles. The 4:1 AR elliptical burner had a higher CO concentration for these profiles due to apparent freezing of the reactions thus it would be expected to have a reduced  $CO_2$  concentration.

The 3:1 AR elliptical burner  $CO_2$  concentration profile for the minor axis was wider than the major axis at the near-burner and midflame, but was narrower at the far-flame profile, indicating an apparent axis switching.

**5.3.5.3 Nitric Oxide:** The turbulent flame (Fig. 5.3.6g to i) had a much reduced peak NO concentration compared to the laminar flame for an equivalence ratio of 4.0. This is due to the reduction of the length of the flame and the five fold increase in jet exit velocity. The turbulent flame was 24% shorter than the laminar for the circular burner, 28% shorter for the 3:1 AR elliptical burner, and 10% shorter for the 4:1 AR elliptical burner. This reduction in length combined with the much greater gas velocity will shorten the residence time significantly, lowering NO production.

For the circular and 3:1 AR elliptical burners, the width of the NO concentration profile was narrower for the turbulent flame for the near-burner and midflame heights and was wider at the far-flame. The turbulent flame from the 4:1 AR elliptical burner had a similar NO concentration profile width as that of the laminar flame for the nearburner and midflame and had a narrower width for the far-flame.

In the turbulent flame, the 3:1 AR elliptical burner tended to produce a greater peak NO concentration than the circular burner for all flame regions. Of note, however, is the observation that for the near-burner and midflame, the minor axis of the 3:1 AR elliptical burner was the primary producer of NO. The major axis NO concentration was negligible along the major axis for the near-burner and midflame regions. At the far flame, the major axis had a higher peak NO concentration than the minor axis. The 4:1 AR elliptical burner produced a much greater peak NO concentration than the circular and 3:1 AR elliptical burners. Again, the 4:1 AR elliptical burner has a greater velocity decay than the circular and 3:1 AR elliptical burners. This higher residence times compared to the circular and 3:1 AR elliptical burners. This higher

residence time offsets the lower temperatures seen in the turbulent flames of the 4:1 AR elliptical burner.

**5.3.5.4 Oxygen:** The oxygen profiles for the turbulent flames of the burners had a similar shape as that of the laminar flames. A core of unreacted oxygen was seen at the centerline of the three burners at the near-burner and mid-flame regions of the flame.

At the far flame, for the three burners, the overall oxygen levels were greater for the turbulent flames compared to the laminar flames. This can be seen in a comparison of the minimum oxygen levels for the flames. The enhanced mixing provided by turbulence was the cause of this. Of particular note is the 4:1 AR elliptical burner which shows much higher  $O_2$  levels in the turbulent flame. This supports the enhanced mixing resulting in freezing of the reactions as noted previously.

The widths of the oxygen deficit regions followed a similar trend as was seen for the CO,  $CO_2$ , and NO concentration profiles. Specifically, the turbulent and laminar flames were similar in width for the near-burner and midflame regions and the turbulent flame was wider at the far-flame.

#### 5.4: Intermediate Species Concentrations

### **5.4.1.1 Hydroxyl Radical Profiles:**

**5.4.1.1 General Observations:** The OH concentration in a flame is an indication of the local intensity of the flame reactions and thus allows an independent determination of the boundary of the flame. The profile figures (Fig. 5.4.1a to c, 5.4.2a to c, 5.4.3a to c, 5.4.4a to c, and 5.4.5a to c) are quantitative in nature while the PLIF images of Section 5.4.2 are qualitative due to the unknown nature of the power distribution of the incident laser light sheet. However the PLIF images will give a good idea of the distribution of the OH radical concentration which should provide insight into the flames.

**5.4.1.2 Effect of Level of Premixing:** For a bulk exit velocity of 20 m/s, at an equivalence ratio of 0.55, the peak concentration of OH in the burners at the near-burner position was much lower than what was seen for the higher equivalence ratios of 1.0 to 4.0. With equivalence ratios of 1.0 to 4.0, at the near-burner, the circular burner peak OH concentration decreased with increase in equivalence ratio, while the 3:1 AR elliptical and 4:1 AR elliptical burners increased in peak OH concentration with increase in equivalence ratio.

At the midflame position, the circular burner had an increase in peak OH concentration with an increase in equivalence ratio from 0.55 to 1.0. The peak OH concentration decreased with increase of equivalence ratio for the circular burner over the range of equivalence ratio of 1.0 to 4.0. The 3:1 AR elliptical burner had a decrease in the peak OH concentration from an equivalence ratio of 0.55 to 1.0 and then increased from 1.0 to 4.0. The 4:1 AR elliptical burner had an increase in peak OH concentration

from equivalence ratios of 0.55 to 1.0 then decreased with a further increase in equivalence ratio to 4.0.

The circular burner peak OH concentration at the far-flame increased from an equivalence ratio of 0.55 to 1.0 then decreased to an equivalence ratio of 4.0. The 3:1 AR elliptical burner increased its peak OH concentration from equivalence ratios of 0.55 to 1.0 and then remained constant until an equivalence ratio of 4.0. The 4:1 AR elliptical burner had a decreased OH concentration with increase in the equivalence ratio of 0.55 to 1.0, increased OH concentration from equivalence ratio of 1.0 to 2.0, and a decreased peak OH concentration with the increase of equivalence ratio from 2.0 to 4.0.

The width of the OH concentration profiles at all heights for all three burners increased with increased equivalence ratio.

**5.4.1.3 Comparison of Circular and 3:1 Aspect Ratio Elliptical Burners:** The circular burner produced a higher peak OH concentration than the 3:1 AR elliptical burner at the near-burner and midflame profiles for equivalence ratios of 1.0 and 2.0. For an equivalence ratio of 4.0, the 3:1 AR elliptical burner produced a greater peak OH concentration compared to the circular burner for all profile heights. Again, as was seen with the temperature and  $CO_2$  concentration data, this increase in OH concentration indicates greater flame intensity. The 3:1 AR elliptical burner also produced a higher peak OH concentration at the far-flame profile for an equivalence ratio of 0.55. All other profiles had similar peak OH concentrations.

All OH concentration profiles for the circular and 3:1 AR elliptical burners showed 'double peak' behavior, although the flame at the midflame and far-flame

profiles of an equivalence ratio of 0.55 had high values of the centerline OH concentrations. In the 3:1 AR elliptical burner flame, the peak OH concentration was located closer to the centerline than in the circular burner for all profiles except for the near-burner with equivalence ratio of 2.0 where the distances from the centerline were similar between the burners.

The OH concentration profiles of the major and minor axes of the 3:1 AR elliptical burner, for an equivalence ratio of 1.0 (Figs. 5.4.5a to c) indicate that the minor axis produced a greater peak OH concentration than the major axis for both the nearburner and midflame profiles. At the far-flame, the peak OH concentrations of the major axis were greater than that of the minor axis. While the major axis OH concentration profile tended to be narrower than that of the circular burner (i.e., the peak concentrations was closer to the centerline), for an equivalence ratio of 1.0, the minor axis OH profile width was very similar to that of the circular burner flame at all three flame profile heights. For an equivalence ratio of 4.0 (Figs. 5.4.6a to c), the peak OH concentrations for the major and minor axis were very similar for the three flame height profiles, with similar profile shapes.

**5.4.1.4 Comparison of 3:1 Aspect Ratio Elliptical and 4:1 Elliptical Aspect Ratio Burners:** For many of the tested equivalence ratio and flame height profiles, the 4:1 AR elliptical burner OH concentration profiles were characterized by a 'triple peak' structure. This triple peak behavior was seen in the lean to stoichiometric flames at the near-burner and midflame profiles and was seen in the rich flames in the mid and far-flame profiles (although the near-burner regions at rich equivalence ratios show a small

centerline concentration of OH). The 3:1 AR elliptical burner produced a higher peak OH concentration for all profiles and equivalence ratios except at the near-burner for equivalence ratios of 0.55, 1.0, and 4.0 and the far-flame profiles of equivalence ratio 2.0 and 4.0 where the peak OH concentrations were similar. Also, at the equivalence ratio of 0.55 midflame and far-flame profiles and the equivalence ratio of 1.0 midflame profile, the 4:1 AR elliptical burner produced a greater peak OH concentration than the 3:1 AR elliptical burner. The peak OH concentrations for the 4:1 AR elliptical burner were located at a greater radial distance from the centerline than for the 3:1 AR elliptical burner.

**5.4.1.5 Turbulence Effects on Burners:** The near-burner and mid flame peak OH concentrations were greater in the laminar flames for the circular and 4:1 AR elliptical burners. The 3:1 AR elliptical burner had similar peak OH concentrations between the laminar and turbulent flames for the near-burner and midflame regions. The circular and 3:1 AR elliptical burners had reduced peak OH concentration at the far-flame of the turbulent flame while the 4:1 AR elliptical burner had similar peak OH concentration at the far-flame of the turbulent flame while the 4:1 AR elliptical burner had similar peak OH concentration between the laminar and turbulent flame.

The turbulent flames tended to have narrower reaction zones than the laminar flame, particularly at the near-burner and midflame. This is seen in the reduction of the width of the OH profiles. This reduction in the reaction zone will tend to reduce the stability of the flame. Of the three burners, the 3:1 AR elliptical burner has the greatest reduction in profile width, which corresponds to its reduced stability as was seen in Chapter 4. For the turbulent flames, the peak OH concentration of the 4:1 AR elliptical burner was lower than that of the other two burners at the near-burner and midflame, and was greater at the far-flame. The reduction in OH was due to freezing of the reactions of the flame as seen in the CO and  $CO_2$  concentration profiles (Sections 5.3.5.1 and 5.3.5.2).

**5.4.2 Hydroxyl Radical Distributions:** Figures 5.4.8a to c show images of the major axis distribution of OH radical concentration of varying equivalence ratio flames with a jet exit velocity of 20 m/s established on each of the burners. These images were created by combining 1 cm wide fields of data taken at overlapping lengths along the flame axis. Again, note that due to difficulties in measuring the power distribution of a laser sheet, these values are qualitative.

With increasing equivalence ratio, the length and width of a core region of little to no OH concentration tended to increase. This corresponds to a jet of unburned fuel air mixture in each flame. The OH concentration boundary for the circular and 3:1 AR elliptical burners was thin for the rich equivalence ratios. In the 4:1 AR elliptical burner, the OH concentration boundary was very thick, particularly at the central regions of the flame. This likely leads to the enhanced stability of the 4:1 AR elliptical burner compared to the 3:1 AR elliptical burner.

#### 5.5: Chapter Conclusions

The enhanced stability of the 4:1 AR elliptical burner (compared to the 3:1 AR elliptical burner) was a result of the presence of a core region of high OH concentration located near the burner exit between the two jets of the 4:1 AR elliptical burner flame and due to a general widening of the OH concentration boundary. This pool of OH radicals stabilizes the flame by enhancing the reaction rates of the flame by increasing the reactivity of the mixture. The OH radical core was further shielded from external disturbances by its location between the two flame jets. This core of OH was created through the interaction of the two flame jets by their close proximity at the near-burner.

In addition, the shorter length of the 4:1 AR elliptical burner allowed more efficient preheating of the reactants. This was seen in the temperature distributions where the unburned fuel cores of the 4:1 AR elliptical burner had a higher gas temperature than the 3:1 AR elliptical burner. This preheating would allow faster reaction rates thus greater stability through flame velocity enhancement. Additionally, stability in the 4:1 AR elliptical burner was increased by a reduction of the core gas velocity of the flame due to an increased velocity decay rate.

The greater values of the normalized RMS of the velocity seen for the 3:1 AR elliptical burner compared to the circular and 4:1 AR elliptical burners confirm the result of Figure 4.1.3 which showed the 3:1 AR elliptical burner transitioning to turbulence earlier to turbulent flow than the circular burner. Again, this was as expected due to the elliptical burners increased turbulence generation. The splitting exhibited by the 4:1 AR elliptical burner tended to reduce the turbulence level of the flame but the turbulence level was still greater than that seen in the circular burner.

The observation in Chapter 4 that the 4:1 AR elliptical burner produced greater CO than the 3:1 AR elliptical and circular burners was a result of the combination of the OH, CO, and temperature profiles. While the 4:1 AR elliptical burner produced lower peak CO concentrations in the profiles, it must be remembered that the emission index is not a function of the *peak* CO produced by a flame but by the *overall* CO production. The 4:1 AR elliptical burner CO distribution was much wider than the other burners thus there was a greater production area for CO. In addition for the 4:1 AR elliptical burner, it was seen that large amounts of CO were present at the edge of the flame. The edge of the flame also had rapidly decreasing temperatures and low OH concentrations (an important radical to the conversion of CO to CO<sub>2</sub>). The combination of drop in temperature and lack of OH leads to the freezing of CO production in the outside edge of the 4:1 AR elliptical burner flame.

The reduced length of the 4:1 AR elliptical burner flames combined with the high flame gas velocities created a much lower residence time for the 4:1 AR elliptical burner compared to the 3:1 AR elliptical and circular burners, thus reducing the NO production for a given jet exit velocity and equivalence ratio. As was seen in Figure 4.4.4, for a given flame length, the 4:1 AR elliptical burner produced a greater emission index of NO than the other burners. The OH radical core may have an enhancing effect on the NO production through the extended Zeldovich reaction (Turns (1996)), which may counteract the shorter residence time.

	Equivalence Ratio	Jet Exit Reynolds Number	Overall Length (cm)	12.5% Length (cm)	25% Length (cm)	50% Length (cm)
4:1 AR El	liptical Burne	er				
20 m/s	0.55	2310	2.82	0.35	0.70	1.41
	1.0	2150	5.04	0.63	1.26	2.52
	2.0	1900	7.05	0.88	1.76	3.52
	4.0	1600	10.7	1.34	2.68	5.37
100 m/s	4.0	7950	9.61	1.20	2.40	4.81

Table 5.1: Axial Location of the Flame Structure Profiles for a 40% by Mass Hydrogen in Propane Flame:

# 3:1 AR Elliptical Burner

20 m/s	0.55	2310	4.28	0.53	1.07	2.14
	1.0	2150	10.0	1.25	2.51	5.02
	2.0	1900	13.5	1.69	3.38	6.77
	4.0	1600	16.7	2.09	4.18	8.36
100 m/s	4.0	7950	12.0	1.50	3.00	6.00

## Circular Burner

20 m/s	0.55	2310	5.94	0.74	1.49	2.97
	1.0	2150	9.76	1.22	2.44	4.88
	2.0	1900	14.6	1.82	3.64	7.29
	4.0	1600	18.2	2.28	4.56	9.10
		_	_		_	_
100 m/s	4.0	7950	13.80	1.73	3.45	6.90

Temperature (K)	EQ = 0.55	EQ = 1.0	EQ = 2.0	EQ = 4.0
Current Study	1849	2173	2173	2084
(laminar)				
Hariharan (2004)	N/A	2050	2100	2000

Table 5.2: Comparison of Peak Temperatures for the 40% by Mass Hydrogen in Propane Flame

Table 5.3: Comparison of Peak Emission Profile Concentrations for the 40% by MassHydrogen in Propane Flame

	Current Study				Hariharan (2004)	
	Laminar			Turbulent	Induced Turbulence	
	EQ = 1.0	EQ = 2.0	EQ = 4.0	EQ = 4.0	EQ = 1.0	EQ = 4.0
CO (%)	7.2	5.5	8.1	3.2	1.4	5
$CO_2$ (%)	3.8	4.5	3.3	4	4	5
NO	32	61	36	12.4	25	100
(ppm)						



Figure 5.1.1a: Maximum Combusting Jet Axial Velocity of the Circular Burner for Jet Exit Velocity of 20 m/s



Figure 5.1.1b: Maximum Combusting Jet Axial Velocity of the 3:1 Aspect Ratio Elliptical Burner for Jet Exit Velocity of 20 m/s







Figure 5.1.1d: Maximum Cold Jet Axial Velocity of the Circular Burner for Jet Exit Velocity of 20 m/s



Figure 5.1.1e: Maximum Cold Jet Axial Velocity of the 3:1 Aspect Ratio Elliptical Burner for Jet Exit Velocity of 20 m/s



Elliptical Burner for Jet Exit Velocity of 20 m/s





Figure 5.1.2f: Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Far-Flame (50% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.1.2g: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Near-Burner (12.5% Flame Length)



Radial Location (r/deff)

Figure 5.1.2h: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Midflame (25% Flame Length)



Figure 5.1.2i: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Far-Flame (50% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.1.2j: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Near-Burner (12.5% Flame Length)



Radial Location (r/deff)

Figure 5.1.2k: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Midflame (25% Flame Length)









for Burner Equivalence Ratio of 1.0 at Far-Flame



Radial Location (r/d<sub>eff</sub>)

Figure 5.1.3g: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)









Figure 5.1.3j: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>) Figure 5.1.3k: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Midflame

(25% Flame Length)



Velocity for Burner Equivalence Ratio of 1.0 at Far-Flame





for Burner Equivalence Ratio of 2.0 at Far-Flame (50% Flame Length)



Radial Location (r/deff)

Figure 5.1.4g: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.1.4h: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Midflame (25% Flame Length)



Figure 5.1.4i: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Far-Flame (50% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.1.4j: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.1.4k: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Midflame (25% Flame Length)



Figure 5.1.4I: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Far-Flame (50% Flame Length)









Radial Location (r/d<sub>eff</sub>)

Figure 5.1.5g: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.1.5h: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 5.1.5i: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Radial Location (r/d<sub>eff</sub>)





Radial Location (r/d<sub>eff</sub>)

Figure 5.1.5k: RMS of Velocity Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)


Circular Burner



Major Axis Minor Axis 3:1 AR Elliptical Burner



Major Axis Minor Axis 4:1 AR Elliptical Burner

## Figure 5.1.6: Schlieren Images of the Three Burners at an Equivalence Ratio of 0.55 with Jet Exit Velocity of 20 m/s

10 mm-

5 mm —

0 mm-







Major Axis Minor Axis 3:1 AR Elliptical Burner



Major Axis Minor Axis 4:1 AR Elliptical Burner

Circular Burner

Figure 5.1.7: Schlieren Images of the Three Burners at an Equivalence Ratio of 1.0 with Jet Exit Velocity of 20 m/s







Major Axis Minor Axis 3:1 AR Elliptical Burner



Major Axis Minor Axis 4:1 AR Elliptical Burner

Circular Burner

Figure 5.1.8: Schlieren Images of the Three Burners at an Equivalence Ratio of 2.0 with Jet Exit Velocity of 20 m/s







Major Axis Minor Axis 3:1 AR Elliptical Burner



Major Axis Minor Axis 4:1 AR Elliptical Burner

**Circular Burner** 

Figure 5.1.9: Schlieren Images of the Three Burners at an Equivalence Ratio of 4.0 with Jet Exit Velocity of 20 m/s



Figure 5.2.1a: Maximum Flame Temperature with Change in Equivalence Ratio at Near-Burner (12.5% Flame Length) for a Jet Exit Velocity of 20 m/s



Figure 5.2.1b: Maximum Flame Temperature with Change in Equivalence Ratio at Midflame (25% Flame Length) for a Jet Exit Velocity of 20 m/s



Figure 5.2.1c: Maximum Flame Temperature with Change in Equivalence Ratio at Far-Flame (50% Flame Length) for a Jet Exit Velocity of 20 m/s













Figure 5.2.4a: Temperature Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)Figure 5.2.4b: Temperature Profiles for Burners at 20 m/s Burner Jet Exit<br/>Velocity for Burner Equivalence Ratio of 2.0 at Midflame<br/>(25% Flame Length)





Figure 5.2.5a: Temperature Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>) Figure 5.2.5b: Temperature Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 5.2.5c: Temperature Profiles for Burners at 20 m/s Burner Jet Ex Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 5.2.6a: Temperature Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/deff) Figure 5.2.6b: Temperature Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)





Figure 5.3.1a Near-Burner (12.5% Flame Length) Peak Carbon Monoxide Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.1b: Midflame (25% Flame Length) Peak Carbon Monoxide

Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.1c: Far-Flame (50% Flame Length) Peak Carbon Monoxide Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.1d: Near-Burner (12.5% Flame Length) Peak Carbon Dioxide Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.1e: Midflame (25% Flame Length) Peak Carbon Dioxide

Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.1f: Far-Flame (50% Flame Length) Peak Carbon Dioxide Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.1g: Near-Burner (12.5% Flame Length) Peak Nitric Oxide Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



**Burner Equivalence Ratio** 

Figure 5.3.1h: Midflame (25% Flame Length) Peak Nitric Oxide Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.1i: Far-Flame (50% Flame Length) Peak Nitric Oxide Concentration with Varying Equivalence Ratio for Jet Exit Velocity of 20 m/s



Figure 5.3.2a: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.3.2b: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Midflame (25% Flame Length)



Figure 5.3.2c: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Far-Flame (50% Flame Length)



Figure 5.3.2d: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Near-Burner (12.5% Flame Length)



Radial Location (r/deff)

Figure 5.3.2e: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Midflame (25% Flame Length)



Figure 5.3.2f: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Far-Flame (50% Flame Length)



Figure 5.3.2g: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Near-Burner (12.5% Flame Length)



Radial Location (r/deff)

Figure 5.3.2h: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Midflame (25% Flame Length)



Figure 5.3.2i: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Far-Flame (50% Flame Length)



Figure 5.3.2j: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Near-Burner (12.5%

Flame Length)



Radial Location (r/d<sub>eff</sub>) Figure 5.3.2k: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Midflame (25% Flame Length)



Figure 5.3.2I: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Far-Flame (50% Flame Length)



Figure 5.3.3a: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)Figure 5.3.3b: Carbon Monoxide Concentration Profiles for Burners at 20 m/sBurner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Midflame (25%<br/>Flame Length)



Figure 5.3.3c: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Far-Flame (50% Flame Length)



Figure 5.3.3d: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.3.3e: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Midflame (25% Flame Length)



Figure 5.3.3f: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Far-Flame (50% Flame Length)



Figure 5.3.3g: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Near-Burner (12.5% Flame Length)



Figure 5.3.3h: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Midflame (25% Flame Length)



Figure 5.3.3i: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Far-Flame (50% Flame Length)





Figure 5.3.4a: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Figure 5.3.4b: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Midflame (25% Flame Length)







Radial Location (r/d<sub>eff</sub>) Figure 5.3.4d: Carbon Dioxide Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Figure 5.3.4e: Carbon Dioxide Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Midflame (25% Flame Length)



Figure 5.3.4f: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Far-Flame (50% Flame Length)



Figure 5.3.4g: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)Figure 5.3.4h: Nitric Oxide Concentration Profiles for Burners at 20 m/sBurner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Midflame (25%<br/>Flame Length)



Figure 5.3.4i: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Far-Flame (50% Flame Length)



Figure 5.3.4j: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>) Figure 5.3.4k: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Midflame (25% Flame Length)



Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Far-Flame (50% Flame Length)



Figure 5.3.5a: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 5.3.5b: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 5.3.5c: Carbon Monoxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



**Radial Location (r/d**<sub>eff</sub>) Figure 5.3.5d: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 5.3.5e: Carbon Dioxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)







**Radial Location (r/d**eff) Figure 5.3.5g: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



**Radial Location (r/d**<sub>eff</sub>) Figure 5.3.5h: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 5.3.5i: Nitric Oxide Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 5.3.5j: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



**Radial Location (r/d**eff) Figure 5.3.5k: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



**Radial Location (r/d**eff) Figure 5.3.5I: Oxygen Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Radial Location (r/d<sub>eff</sub>) Figure 5.3.6a: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



**Radial Location (r/d**<sub>eff</sub>) Figure 5.3.6b: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



**Radial Location (r/d**eff) Figure 5.3.6c: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



 $\begin{array}{c} \textbf{Radial Location (r/d_{eff})} \\ \textbf{Figure 5.3.6d: Carbon Dioxide Concentration Profiles for Burners at 100 m/s} \\ \textbf{Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner} \end{array}$ 





**Radial Location (r/d**eff) Figure 5.3.6e: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



**Radial Location (r/d**<sub>eff</sub>) Figure 5.3.6f: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Radial Location (r/d<sub>eff</sub>)Figure 5.3.6g: Nitric Oxide Concentration Profiles for Burners at 100 m/sBurner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner(12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.3.6h: Nitric Oxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



**Radial Location (r/d**eff) Figure 5.3.6i: Nitric Oxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



**Radial Location (r/d**eff) Figure 5.3.6j: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)Figure 5.3.6k: Oxygen Concentration Profiles for Burners at 100 m/s BurnerJet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame



Figure 5.3.6I: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 5.4.1a: Near-Burner (12.5% Flame Length) Peak Hydroxyl Radical Concentration with Varying Equivalence Ratio For Jet Exit Velocity of 20 m/s



Figure 5.4.1b: Midflame (25% Flame Length) Peak Hydroxyl Radical Concentration with Varying Equivalence Ratio For Jet Exit Velocity of 20 m/s



Figure 5.4.1c: Far-Flame (50% Flame Length) Peak Hydroxyl Radical Concentration with Varying Equivalence Ratio For Jet Exit Velocity of 20 m/s



Figure 5.4.2a: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Near-Burner (12.5% Flame Length)



Figure 5.4.2b: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Midflame (25% Flame Length)



Figure 5.4.2c: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 0.55 at Far-Flame (50% Flame Length)



Figure 5.4.3a: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Near-Burner (12.5% Flame Length)



Figure 5.4.3b: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Midflame (25% Flame Length)



Figure 5.4.3c: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 1.0 at Far-Flame (50% Flame Length)


Radial Location (r/deff)

Figure 5.4.4a: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.4.4b: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Midflame (25% Flame Length)



Figure 5.4.4c: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 2.0 at Far-Flame (50% Flame Length)



Radial Location (r/deff)

Figure 5.4.5a: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/deff)

Figure 5.4.5b: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 5.4.5c: Hydroxyl Radical Concentration Profiles for Burners at 20 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.4.6a: Hydroxyl Radical Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Radial Location (r/d<sub>eff</sub>)

Figure 5.4.6b: Hydroxyl Radical Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 5.4.6c: Hydroxyl Radical Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



m/s with Varying Jet Exit Equivalence Ratio



Figure 5.4.8b: PLIF Images of OH Radical Concetration Distribution of the 3:1 AR Elliptical Burner with Jet Exit Velocity of 20 m/s with Varying Jet Exit Equivalence Ratio



Figure 5.4.8c: PLIF Images of OH Radical Concentration Distribution of the 4:1 AR Elliptical Burner with Jet Exit Velocity of 20 m/s with Varying Jet Exit Equivalence Ratio

#### **CHAPTER 6: COMPUTATIONAL RESULTS**

#### 6.1: Computational Flame Structure

**6.1.1 General Notes:** Computationally, turbulent flames from a circular and a 3:1 AR elliptical burners were modeled using the Computational Fluid Dynamics (CFD) package, FLUENT version 6.1.22. Only turbulent flames will be considered for this study due to turbulent flames being the most common flames in practical use and thus more likely to be simulated. A mixture of 40% by mass hydrogen in propane fuel premixed with air was used in this study. The flames studied had a burner exit velocity of 100 m/s (Re = 7950) and were rich partially premixed with an equivalence ratio of 4.0.

The circular burner was modeled using a 2-D axisymetric domain (Figure 6.1.1). This overall grid had dimensions of 40 cm in length and 3 cm radial distance. For the 3:1 AR elliptical burner, the computational model was solved using a three-dimensional structured domain (required since, due to the aspect ratio of the 3:1 AR elliptical burner, the flow is nonaxisymmetric) of a quarter cylinder with a radius of 3 cm and a total length of 20 cm (Fig. 6.1.1). The center of the radius of the cylinder was located at the center of the burner exit with planes of symmetry aligned to the major and minor axis of the burner. This assumes that the flow field, while not axially symmetric, will be symmetric about the major and minor axis.

The flame modeled was for a burner exit velocity of 100 m/s with a 40% by mass hydrogen in propane fuel mixture. The dimensions of the burners of the experimental study were used for the computational model; the circular burner had a 2 mm diameter and the 3:1 burner was modeled with major axis dimensions of 3.4 mm and minor axis diameter of 1.2 mm. The flame was premixed to an equivalence ratio of 4.0 at the burner exit.

The reacting jets were simulated with three models: a k- $\varepsilon$  turbulence model with a probability density function (PDF) approach to modeling the reacting flow, a seven equation Reynolds Stress Model (RSM) with an eddy dissipation model, and the RSM with an Eddy Dissipation Concept (EDC) model for the combusting flow. For the eddy dissipation and EDC, a four-step global reaction model was used.

Appropriate settings used for modeling with the FLUENT code are given in Tables 6.1.1 to 6.1.6b.

**6.1.2 Global Reaction Model:** For the CFD computations, a reduced kinetics model was used to simulate the combustion. A complex kinetics model such as that of Qin, et al. (2000) was not used due to the extreme computational expense involved, particularly for the 3-dimensional 3:1 AR elliptical burner grid. To simply the chemical calculations, a two step propane-oxygen (with reversible reaction) reduced kinetics model by Westbrook and Dryer (1981) was combined with a single step hydrogen-oxygen global reaction by Marinov et al. (1999). The steps and reaction rate parameters of this model are given in Table 6.1.1. The propane mechanism was previously used successfully to predict flame properties by Ye et al. (2004), is listed in Turns (1996) as a 'standard' model, and is one of the default propane combustion models in the FLUENT code. The hydrogen model used gives a good prediction of the hydrogen air flame speed.

**6.1.3 Grid Development:** Initially, a very coarse grid of 6 cells/cm radially and 3 cells/cm axially was used for the 3:1 AR elliptical burner. This was chosen to reduce the initial computational time of the solution. When a solution was found for this coarse grid, a refinement of the grid was made at the near burner region of the flame. The solution was then rerun for this new grid. This iterative process was repeated twice more. The results of this grid refinement procedure are given in Figures 6.1.3.1 to 6.1.3.2c. These results are for the RSM model with EDC for the major axis of the 3:1 AR elliptical burner.

The greatest difference in the profiles occurred from the transition from the original grid to the first adaptation shown in Fig. 6.1.3.2a to c. There was a dramatic shift of the radial location of the peak temperature at the near-burner and a general increase in the magnitude of the peak flame temperature at the midflame and far-flame profiles. With increasing grid density the differences in the change in magnitude and radial position of the maximum temperature become small (less that 50 K or 0.5 mm). Thus the solution has become reasonably grid independent for the highest adaption.

A similar adaptation was performed with the circular burner with similar results.

**6.1.4 Combustion**\**Turbulence Model Development**: In order to determine the best trade-off of computational complexity with accurate results, the flame was simulated with three computational models: a k- $\varepsilon$  turbulence model in conjunction with a Probability Distribution Function (PDF) method to simulate combustion, a Reynolds Stress Model (RSM) for turbulence with an eddy dissipation combustion model, and a RSM with a eddy dissipation concept (EDC) combustion model. The theory behind these models is

given in Appendix C. Figures 6.1.4.1 through Fig 6.1.4.12c give the results of these three models compared to experimental measurements.

The k- $\varepsilon$  turbulence model with a PDF model produced a flame with a much shorter inner unreacted cone and reduced peak temperatures (particularly at the nearburner) than was seen in the experimental results. Also, the k- $\varepsilon$  turbulence model with PDF tended to greatly overestimate the CO concentration and underestimate the CO<sub>2</sub> concentration profiles with very poor matching of the location of the peak concentrations. These errors were seen for both the circular and 3:1 AR elliptical burners.

The RSM turbulence model with eddy dissipation simulated combustion somewhat better than the k- $\epsilon$  turbulence model with PDF. The peak flame temperatures and locations were better matched with experimental data and the radial locations of the peaks in the CO concentration profiles were reasonably matched. However, this model, like the k- $\epsilon$  turbulence model with PDF tended to dramatically over predict the CO and under predict the CO<sub>2</sub> concentration profiles. Also, a multiple peak structure was seen with the CO<sub>2</sub> which was not present in the experimental results.

The Reynolds Stress model with an Eddy Dissipation Concept (EDC) model had much greater predictive success than the previous two models with good matching of both the magnitude and location of the temperature, CO concentration, and CO<sub>2</sub> concentration peaks, particularly in the near-burner region. Therefore, this was the model used for the final results for both the 2-dimensional circular burner model and the 3dimensional 3:1 AR elliptical burner.

# 6.1.5 Results:

**6.1.5.1 General Observations:** The temperature, velocity, mole fraction of species, and reaction rate distributions developed by the RSM turbulence model with EDC combustion modeling are shown in Figures 6.1.5.1 to 6.1.5.13.

The reaction rate of the hydrogen consumption reaction (Reaction 4 as shown in Fig. 6.1.5.13) is several orders of magnitude greater than that of the propane consumption reaction (Reaction 1 in Fig. 6.1.5.10). This is a consequence of the fast reactivity of the hydrogen reaction depleting the available premixed oxygen. The combustion of hydrogen occurs first in the model and this very quickly consumes the oxygen in the fuel/air mixture. This propane consumption rate is then limited by the availability of oxygen which has to be supplied my mixing with the surrounding air. This dramatically reduces the reaction rate of the propane consumption.

**6.1.5.2 Comparison of Circular and 3:1 AR Elliptical Burner:** The 3:1 AR elliptical burner flame was shorter in length than the flame of the circular burner based on the distributions, i.e., the peak temperature and species concentrations of the flame occurred at a shorter axial distance from the burner. This is in agreement with the flame length results seen in Chapter 4.

An axis switching was seen in the 3:1 AR elliptical burner velocity distribution at an axial distance of 3.9 cm (19.5  $x/d_{eff}$ ). This is close to the axis switching seen by Gollahalli et al. (1992) which occurred at 20  $x/d_{eff}$  for a turbulent diffusion flame. This indicates that there is a rapid growth of the minor axis and much slower growth with the major axis. This will have an effect on the mixing of the jet. This effect of mixing is easily seen in the  $N_2$  concentration distribution (Fig. 6.1.5.9). For the reaction model, nitrogen was an inert substance so changes in the field of the  $N_2$  concentration distribution will be primarily a function of the mixing of the jet (which has a lower nitrogen concentration) with the atmospheric air. There will also be a small effect of the changing total moles of gas due to reactions. Examining the nearburner we can see that the  $N_2$  concentration gradient is narrower on the major axis than the minor axis. This implies greater mixing of the ambient air into the jet along the major axis than the minor axis. The mixing results are in good agreement with Ho and Gutmark (1987) who found on the major axis plane that the shear layer of the jet spread into the potential core while on the minor axis, the shear layer spread out into the surrounding air.

The mixing characteristics that cause the axis switching resulted in the minor axis of the 3:1 AR elliptical burner having a broader flame zone than the major axis at the near burner region. This is seen with in the wide temperature, CO, CO<sub>2</sub>, O<sub>2</sub> and H<sub>2</sub>O concentration distributions along the minor axis (Fig, 6.1.5.1, Fig. 6.1.5.3 to 6.1.5.5, and Fig. 6.1.5.8). The propane in the unburned fuel core tended to exist to a greater radial distance from the centerline for the minor axis when compared to the major axis, due to the expansion of the core into the surrounding air.

Evidence indicating that the hydrogen reaction (Reaction 4) consumes all the available premixed air can be seen in Fig. 6.1.5.13. This figure shows that are two regions where hydrogen reactions are occurring. The strongest reaction of  $H_2$  occurs in a cone located at the burner exit to an axial distance of over 5 cm in the circular burner and 5 cm for the elliptical burner. This reaction region would correspond to the hydrogen combustion the premixed air. A second region is seen by the presence of a less intense

hydrogen reaction rate occurring in a hollow ended cylinder starting at a axial distance of about 2 cm for both flames and continuing to an axial height of 6.5 cm for the circular burner and 6 cm for the 3:1 AR elliptical burner. This corresponds to a reaction zone where remaining hydrogen after the premix reaction mix and react with the surrounding air.

The propane consumption reaction zone (Reaction 1), CO consumption reaction zone (Reaction 2), and the  $CO_2$  dissociation regions of the 3:1 AR elliptical burner are broader in width and less intense than those seen in the circular burner, particularly in the midflame and far-flame regions. This is a result of the enhanced mixing of the 3:1 AR burner distributing the reactions.

## 6.2: Post Gas Reaction Freezing Studies

It was proposed in Chapter 4 that the increased CO production of the 4:1 AR elliptical burner compared to the circular and 3:1 AR elliptical burners was due to increased mixing with ambient air. This mixing decreased the temperature of the flame gases and, in addition, diluted the post flame gases. This temperature reduction freezes the CO to  $CO_2$  reaction pathways thus increasing the final CO concentration. To test this theory, this reaction freezing was simulated computationally to determine the conditions at which increased CO production would occur and compare to conditions seen experimentally.

**6.2.1 Model Conditions:** For the detailed reaction model, this study uses the model of Qin et al. (2000). This model was chosen because it is a moderately detailed reaction mechanism (70 species, 463 reactions) capable of  $C_2/C_3$  hydrocarbons that has been shown to predict well the laminar flame speeds of hydrocarbon/hydrogen mixtures of methane, ethylene, and propane (Law and Kwon (2004)). The model has detailed carbon and hydrogen combustion pathways which allow its use with hydrogen/hydrocarbon/air mixtures.

To perform validation of the kinetics model of Qin et al. (2000), the Premix module of the Chemkin Collection 3.7 was used. The theory used by Chemkin in its calculations is given in Appendix D. A detailed listing of the elementary reactions and Arrhenius parameters of the model by Qin et al. (2000) is given in Appendix E in a Chemkin compatible input format. A format sample of the the input file to Chemkin is given in Appendix F. **6.2.2 Validation of Model:** In order to see if the chosen kinetics model accurately models the flames of the study, the laminar flame speed predictions of the model were compared to the established flame speed literature.

Initially, the values of flame speed of the pure fuel cases were computed. Plotted are figures showing the laminar flame speed of hydrogen/air flames (Fig. 6.2.2.1a) and propane/air flames (Fig. 6.2.2.1b) with variation of equivalence ratio. The computational laminar flame speed for the propane only premixed flame matched the experimental flame speeds of Turns (1996), Kanury (1975), Zhao et al. (2004), and Vagelopoulos and Egolfopoulos (1998) very well. The Qin et al. (2000) model was optimized for propane combustion, therefore this was not unexpected. However, despite the model being optimized for propane/air flames, there is a good match to the hydrogen/air flame speeds of Turns (1996), Kanury (1975), Chen and Bilger (2000), Im and Chen (2000), and Aung et al (1997), with the model under predicting the laminar flame speed for lean mixtures. This implies that hydrocarbon/hydrogen mixtures should be well modeled by the kinetics model of Qin et al (2000).

As a further validation, the values of the flame speed for varying mole fractions of propane in hydrogen fuel were computed. A lean, stoichiometric, and fuel rich flame were modeled. Figure 6.2.2.2 confirms that the predicted flame speed of the propane/hydrogen/air premixed flame agrees with the experimental results of Law and Quon (2004). The model predicts the stoichiometric and rich mixture laminar flame speeds well, but, at very low  $C_3H_8$  mole fractions, under predicts the flame velocity for the lean mixture. The mole fraction of propane in the present study was 0.06, which

appears to be reasonably modeled. Therefore, this model should predict the detailed kinetics in hydrogen/propane flames well.

**6.2.3: Results:** Figures 6.2.3.1 and 6.2.3.2 show the effect of varying hydrogen mass percentages on the flame properties. Increasing the hydrogen percentage increases the adiabatic flame temperature for a given equivalence ratio with a greater effect seen for rich flames. Increasing the hydrogen percentage increases the flame speed and linearly shifts the location of the maximum flame speed to richer mixtures.

To study of the effect of freezing of the CO reactions on the CO production of propane/hydrogen premixed flames, the above reaction scheme of Qin et al. was used with the Chemkin code. Initially, the freely propagating flame solution was found for a 40% by mass  $H_2$  in  $C_3H_8$  mixture at an equivalence ratio of 1.0. The freely propagating flame solution simulates the 1-dimensional propagation of flame through a homogenous fuel air mixture. No restrictions were made on the temperature profile. After the computation, the temperature, CO concentration, and OH concentration profiles were then extracted and plotted (Fig. 6.2.3.3a to c).

To simulate freezing of the flames, the temperature profile of the freely propagating flame was used as a temperature profile for a 'burner stabilized' flame in Chemkin. In a 'burner stabilized' run, the temperature profile is set by the user and the chemical reactions are calculated given this fixed temperature profile. With the temperature profile of the freely propagating flame solution input as the fixed temperature profile, it was found that the burner stabilized case was the same as the initial freely propagating flame.

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To simulate the effects of mixing of the cooler quiescent environment with the combusting gases, the temperature profile was modified so that, shortly after the flame front (as determined by the location of maximum carbon monoxide), the gas temperature was cooled to that of the surrounding atmosphere (300K) at variable rates defined by the imposed temperature gradient in units of K/mm (Figure 6.2.3.3a). The reaction model was then run with these modified temperature profiles and the temperature modified CO and OH concentration distributions were extracted and plotted.

From this modeling, initially two regions were seen in the results (Table 6.2.1 and Figures 6.2.3.3b to c). For drops in temperature of 400 K/mm or less, the CO concentration of the flame at a position 3 cm downstream of the flame front was less than that of the non-quenched flame. For drops more rapid than 400 K/mm, the 'final' CO concentration was greater than the unquenched flame. However, these two regions are an artifact of the comparison. For a real comparison of the CO production of a flame the CO concentration is usually measured at a location where the flame gases have cooled to close to atmospheric values. For the 'no freezing' case, the flame gases at the end of the flame front are near the adiabatic flame temperature. This high temperature causes a dissociation of the CO concentration will naturally decrease. For a better comparison of the CO production, the 100 K/mm temperature drop case should be used as the indication of the final CO concentration of a real flame. In this case, greater rates of decrease in temperature cause greater amounts of final CO in the cooled post combustion gases.

It becomes apparent from Fig. 6.2.3.3c that OH is a strong indicator of the freezing of the CO to  $CO_2$  reactions. In all cases, the CO concentration reached a steady

state value when the OH mole fraction became negligible. An examination of the data indicates that this freezing occurred when the flame gases had a temperature of 1000K or less.

From Chapter 5, it was noted that the 4:1 AR elliptical burner had regions on the outside edges of the flame that exhibited significant CO concentration, low OH concentrations and rapidly decreasing temperatures. From the results of the computational study, it would appear that these regions were the cause of the increased  $EI_{CO}$  of the 4:1 AR elliptical burner (compared to the circular and 3:1 AR elliptical burners) seen in Chapter 4.

# 6.3: Chapter Conclusions

It was found that 40% hydrogen by mass in propane partially premixed flames from circular and 3:1 AR elliptical burners could be reasonably accurately modeled with FLUENT code if a Reynolds Stress Model (RSM) with a Eddy Dissipation Concept (EDC) combustion model with a four-step kinetics model is used. The model accurately predicted the CO and CO<sub>2</sub> concentration profiles and modeled the temperature profiles of the flames reasonably well, particularly at the near-burner and midburner regions.

The model found that the minor axis had a broader flame zone (indicated by the temperature and species profiles) than the major axis. An examination of the axial velocity and nitrogen concentration distributions linked this broadening of the flame zone to the axis switching seen in elliptical burners. The major axis tended to entrain ambient air inwards while the minor axis tended to spread the fuel core outwards. This gave the major axis better  $O_2$  entrainment thus creating narrower flame zones.

It was also found from a detailed chemical kinetic model, that rapid reductions in the post flame gases of 40% by mass hydrogen in propane premixed flames can freeze the CO to  $CO_2$  reaction pathways, thus increasing the overall emission of CO from a flame. From Chapter 4 and 5, it was identified that the 4:1 AR elliptical burner had increased EI<sub>CO</sub> compared to the circular and 3:1 AR elliptical burners, and that this increase in CO production was likely due to regions of high CO concentration, low temperature, and negligible OH concentrations in the periphery of the flame. The detailed kinetic model provides support for this explanation.

Reaction 1:	Reaction 2:			
c3h8 + 3.5 o2 => 3 co + 4 h2o	co + 0.5 o2 => co2			
A = 5.62e09	A = 2.239e12			
Ea = 1.256e08 (j/kgmol)	Ea = 1.7e08 (j/kgmol)			
$[c3h8]^{0.1}$ $[o2]^{1.65}$	$[co]^1$ $[o2]^{0.25}$ $[h2o]^{0.5}$			
Reaction 3:	Reaction 4:			
Reaction 3: $co2 \Rightarrow co + 0.5 o2$	Reaction 4: h2 + 0.5 o2 => h2o			
Reaction 3: co2 => co + 0.5 o2 A = 5e08	Reaction 4: h2 + 0.5  o2 => h20 A = 9.87e08			
Reaction 3: co2 => co + 0.5 o2 A = 5e08 Ea = 1.7e08 (j/kgmol)	Reaction 4: h2 + 0.5  o2 => h20 A = 9.87e08 Ea = 3.1e07 (j/kgmol)			

Table 6.1.1: Kinetics Model for Flow Field Modeling (FLUENT)

Table 6.1.2: Relaxation Parameters

Pressure = 0.3Density = 1Body Forces = 1Momentum = 0.7Turbulence Kinetic Energy = 0.8**Turbulence** Dissipation Rate = 0.8Turbulent Viscosity = 1**Reynolds Stresses 0.5** c3h8 = 1 $o^2 = 1$ co2 = 1co = 1h2o = 1h2 = 1Energy = 1

# Table 6.1.3: Discretation Methods

Pressure: Standard Pressure –Velocity Coupling: SIMPLE Momentum: First Order Upwind Turbulence Kinetic Energy: First Order Upwind Turbulence Dissipation Rate: First Order Upwind Reynolds Stresses: First Order Upwind c3h8: First Order Upwind o2: First Order Upwind co2: First Order Upwind co2: First Order Upwind h2o: First Order Upwind h2: First Order Upwind Energy: First Order Upwind

Table 6.1.4: H	Reynolds	Stress (	(7 Eq	uation	) Model	Input
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Reynolds-Str	ess Options:
	Wall B. C. from k Equation: On
	Quadratic Pressure-Strain Model: Off Wall Reflection Effects: On
Near-Wall Tr	reatment:
	Standard Wall Functions
Options:	
	Viscous Heating: off
Model Consta	ants: (default)
	Cmu = 0.09
	C1-Epsilon = 1.44
	C2-Epsilon = 1.92
	C1-PS = 1.8
	C2-PS = 0.6
	C1'-PS = 0.5
	C2' - PS = 0.3
	TKE Prandtl Number = 1
	TDR Prandtl Number = $1.3$
	Energy Prandtl Number = 0.85
	Wall Prandtl Number = $0.85$
	Turn Schmidt Number = $0.7$

Table 6.1.5: Species Transport Model

Reactions: Volumetric			
Integration Parameters:			
Integration Options: ISAT			
ODE parameters:			
Absolute Error Tolerance = $1e-06$			
Relative Error Tolerance = 1e-09			
Integration parameters			
ISAT Error Tolerance $= 0.001$			
Max. Storage $(Mb) = 100$			
Reference Time Step $(s) - 0.001$			
Number of Trees $= 4$			
Verbosity = 0			
Options:			
Diffusion Energy Source: On			
Full Multicomponent Diffusion: Off			
Thermal Diffusion: Off			
Mixture Properties			
Mixture Material:			
propane-h2-air-2step			
Turbulence-Chemistry Interaction: EDC			
EDC Options:			
Volume Fraction Constant = $2.1377$			
Time Scale Constant = $0.40825$			
Flow Its. Per Chem. Update = $10$			

Table 6.1.6.a: Boundary Conditions

Burner Top	
Wall	Adiabatic (0 W/m2)
	Stationary
	No Slip
	Roughness Height = $0 \text{ m}$
	Roughness Constant = $0.5$
	No Surface Reaction
	No species flux
"Coflow"	
Pressure-Inlet	Gauge Total Pressure = 5 Pa
	Supersonic/Initial Gauge Pressure (pascal) = 0
	Total Temperature $(K) = 300$
	Direction Specification Method: Normal to Boundary
	Turbulence Specification Method: K and Epsilon
	Turb. Kinetic Energy $(m2/s2) = 0$
	Turb. Dissipation Rate $(m2/s3) = 0$
	Reynolds-Stress Specification Method: K or Turbulence Intensity
	Species Mass Fractions:
	c3h8 = 0
	o2 = 0.23
	co2 = 0
	co = 0
	h2o = 0
	h2 = 0

Table 6.1.6.b: Boundary Conditions

majsym, minsym	n, symmetry			
Symmetry				
<u> </u>				
outflow, outside				
Pressure-Outlet	Gauge Pressure (Pa) = $0$			
	Radial Equilibrium Pressure Distribution: Off			
	Backflow Total Temperature $(K) = 300$			
	Backflow Direction Specification Method: Normal to Boundary			
	Turbulence Specification Method: K and Epsilon			
	Turb. Kinetic Energy $(m2/s^2) = 0$			
	Turb Dissipation Rate $(m^2/s^3) = 0$			
	Reynolds-Stress Specification Method: K or Turbulence			
	Intensity			
	Species Mass Fractions			
	c3h8 = 0			
	o2 = 0.23			
	co2 = 0			
	co = 0			
	h2o = 0			
	h2 = 0			
Inlet				
<b>X7 1</b> 4 <b>X 1</b> 4	Velocity Specification Method: Magnitude, Normal to			
<u>Velocity Inlet</u>	Boundary			
	Reference Frame: Absolute			
	Velocity Magnitude $(m/s) = 100$			
	Temperature (K) = $300$			
	Turbulence Specification Method: K and Epsilon			
	Intensity			
	Spacies Mass Eractions:			
	$\frac{3}{2}$ $\frac{3}$			
	$c_{310} = 0.000000000000000000000000000000000$			
	02 = 0.190039			
	$c_{02} = 0$			
	$b^{2}c = 0$			
	$h_{20} = 0$ h_2 = 0.05006228			
	h2 = 0.05906238			

Temperature Drop	Mole Fraction of CO in End Gases	Temperature Drop	Mole Fraction of CO in End
			Gases
No Freezing	0.0043	400 K/mm	0.004286
100 K/mm	0.0010	500 K/mm	0.005098
200 K/mm	0.0024	1000 K/mm	0.00631
300 K/mm	0.0035		

Table 6.2.1: Final CO Concentrations of Freezing Cases



Figure 6.1.1: Schematic of Computational Domain



Figure 6.1.3.1: Variation of Grid for Sensitivity 3:1 Burner Grid - Major Axis Plane



Figure 6.1.3.2a: Temperature Variation with Grid Size for the Near-Burner Major Axis of the 3:1 AR Elliptical Burner



Figure 6.1.3.2b: Temperature Variation with Grid Size for the Midflame Major Axis of the 3:1 AR Elliptical Burner



Figure 6.1.3.2c: Temperature Variation with Grid Size for the Far-Flame Major Axis of the 3:1 AR Elliptical Burner







Figure 6.1.4.2a: Temperature Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.2b: Temperature Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame

(50% Flame Length)



Figure 6.1.4.3a: Temperature Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.3b: Temperature Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 6.1.4.4a: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.4b: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.4c: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 6.1.4.5a: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.5b: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.5c: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 6.1.4.6a: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.6b: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.6c: Carbon Monoxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 6.1.4.7a: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.7b: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.7c: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Radial distance (r/d)

Figure 6.1.4.8a: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.8b: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.8c: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Radial distance (r/d)

Figure 6.1.4.9a: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.9b: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.9c: Carbon Dioxide Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)


Figure 6.1.4.10a: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.10b: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.10c: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 6.1.4.11a: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.11b: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.11c: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Radial distance (r/d)

Figure 6.1.4.12a: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Near-Burner (12.5% Flame Length)



Figure 6.1.4.12b: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Midflame (25% Flame Length)



Figure 6.1.4.12c: Oxygen Concentration Profiles for Burners at 100 m/s Burner Jet Exit Velocity for Burner Equivalence Ratio of 4.0 at Far-Flame (50% Flame Length)



Figure 6.1.5.1: Comparison of the Computational Temperature Field of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.2: Comparison of the Computational Axial Velocity Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.3: Comparison of the Computational CO Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.4: Comparison of the Computational CO<sub>2</sub> Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.5: Comparison of the Computational O<sub>2</sub> Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.6: Comparison of the Computational  $C_3H_8$ Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.7: Comparison of the Computational H<sub>2</sub> Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.8: Comparison of the Computational  $H_2O$ Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.9: Comparison of the Computational N<sub>2</sub> Distribution of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.10: Comparison of the Computational Reaction Rate of Reaction 1 of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.11: Comparison of the Computational Reaction Rate of Reaction 2 of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.12: Comparison of the Computational Reaction Rate of Reaction 3 of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.1.5.13: Comparison of the Computational Reaction Rate of Reaction 4 of a Circular and a 3:1 AR Elliptical Burner with 40% by Mass Hydrogen in Propane Flame of Jet Exit Velocity of 100 m/s



Figure 6.2.2.1a: Validation of Full Model Laminar Flame Speed Results for Hydrogen/Air Premixed Flames



Figure 6.2.2.1b: Validation of Full Model Laminar Flame Speed Results for Propane/Air Premixed Flames



Figure 6.2.2.2: Validation of Effect of Increasing Mole Fraction of Propane on Flame Speed



Figure 6.2.3.1: Equilibrium Flame Temperatures



Figure 6.2.3.2: Equivalence Ratio Effect on Laminar Flame Speed for Gas Mixtures



Figure 6.2.3.3a: Axial Flame Temperature Profiles for CO Quenching Experiments



Figure 6.2.3.3b: Axial CO Concentration Profiles for CO Quenching Experiments



Figure 6.1.3.3c: Axial OH Concentration Profiles for CO Quenching Experiments

#### **CHAPTER 7: SUMMARY AND CONCLUSIONS**

### 7.1: Summary of Results

This study was an investigation of the properties of premixed flames generated from elliptical burners. Three burner geometries were used: a circular nozzle of exit inside diameter 2.0 mm, a 3:1 aspect ratio elliptical nozzle of exit inside dimensions 3.4 mm for the major axis by 1.2 mm for the minor axis, and a 4:1 aspect ratio elliptical nozzle with exit inside dimensions of 4.0 mm for the major axis and a 1.0 mm for the minor axis. Mixtures of propane and hydrogen were used as the fuel.

The blow out velocity was increased with increase in hydrogen mass fraction of the hydrogen/propane fuel mixture. For burner exit equivalence ratios of 1.0 and greater, the circular burner was able to attain a higher blow out velocity than the elliptical burners. For the elliptical burners, the 4:1 AR elliptical burner had a higher blow out velocity than the 3:1 AR elliptical burner. For equivalence ratios less than 1.0, the maximum blow out velocity for the three burners was similar.

From the stability results, a fuel mixture of 40% hydrogen by mass in propane was chosen in order to allow a broad range of attached burner velocities (Reynolds numbers) in order to see the differences between laminar and turbulent flames issuing from the elliptical burners.

For the three burners of the study, the circular burner transitioned to a turbulent flame at the highest critical Reynolds number, the 3:1 AR elliptical burner at the lowest, and the 4:1 AR elliptical burner transitioned at a critical Reynolds number intermediate to the two other burners. It is known that elliptical burners exhibit higher turbulence levels

than circular burners, thus the lower critical Reynolds number. The 4:1 AR elliptical burner has an increased velocity decay rate that reduces the turbulence generation, thus it transitions later than the 3:1 AR elliptical burner. The critical Reynolds number of the circular burner increased with an increase in burner exit equivalence ratio while the critical Reynolds numbers of the elliptical burners were insensitive to changes in the equivalence ratio. The RMS of the velocity (a measure of turbulence) of the burners confirmed this result.

The flames of this study visually consisted of two regions: a bright blue inner cone corresponding to a premixed flame and a dim bluish outer flame corresponding to a diffusion type flame where uncompleted reactions in the premixed flame continue.

The laminar flames of the 3:1 AR elliptical and circular burners, for varying equivalence ratio corresponding to a jet exit velocity of 20 m/s, were similar in appearance and overall flame length. The laminar 4:1 AR elliptical burner split into two sub-flames along the burner major axis. This splitting had the effect of greatly shortening the 4:1 AR elliptical flame to an overall flame length of only about half that of the circular and 3:1 AR elliptical flames. The length of both flame regions increased with increasing burner exit equivalence ratio.

For laminar flames, the 3:1 AR elliptical and circular burners produced similar carbon monoxide and nitric oxide emission indexes over the range of equivalence ratios of 0.55 to 4.0. The 4:1 AR elliptical burner produced greater CO and lower NO emission indexes than the other two burners for laminar flames. For all burners an increase in equivalence ratio tended to decrease the production of CO and increase the production of NO.

For turbulent flames, both of the elliptical burners tended to produce more CO and less NO than the circular burner, with the difference between the elliptical and circular burner emission production being greater at an equivalence ratio of 2.0.

### 7.2: Conclusions

The enhanced stability of the 4:1 AR elliptical burner (compared to the 3:1 AR elliptical burner) was a result of the presence of a core region of high OH concentration located near the burner exit between the two jets of the 4:1 AR elliptical burner flame and due to a general widening of the OH concentration boundary. This pool of OH radicals stabilized the flame by enhancing the reaction rates of the flame. The core of OH radicals was further shielded from external disturbances by its location between the two flame jets. This core of OH was created through the interaction of the two flame jets by their close proximity at the near-burner. In addition, the shorter length of the 4:1 AR elliptical burner allowed more efficient preheating of the reactants. This was seen in the temperature distributions where the unburned fuel cores of the 4:1 AR elliptical burner had a higher gas temperature than the 3:1 AR elliptical burner. This preheating allowed faster reaction rates thus greater stability through flame velocity enhancement. Additionally, stability in the 4:1 AR elliptical burner was increased by a reduction of the core gas velocity of the flame due to an increased velocity decay rate.

The increase in production of CO by the 4:1 AR elliptical burner was a result of a combination of the OH, CO, and temperature profiles. In the 4:1 AR elliptical burner, large amounts of CO were present at the edge of the flame. The edge of the flame had rapidly decreasing temperatures and low OH concentration (an important radical to the conversion of CO to  $CO_2$ ). The combination of drop in temperature and lack of OH led to the freezing of CO production in the outside edge of the 4:1 AR elliptical burner flame as was shown in the computational results.

The reduced length of the 4:1 AR elliptical burner flames created a much lower residence time for the 4:1 AR elliptical burner compared to the 3:1 AR elliptical and circular burners thus reducing the NO production. For a given flame length, the 4:1 AR elliptical burner produced a greater emission index of NO than the other burners. The OH radical core might have an enhancing effect on the NO production through the extended Zeldovich reaction (Turns (1996)), which counteracted the shorter residence time.

### 7.3: Practical Implications

The main practical implication of this study is that the use of elliptical burners with premixed flames does not increase the stability of turbulent flames where the flame issues into a quiescent environment. This means that circular burners are still preferable to elliptic geometries for ultra lean concept (ULC) burners at least for inlet velocity blowout.

Elliptical burners would be most useful in designs that require a short flame length. For laminar flames, a reduction by half of the burner length is possible if a 4:1 AR elliptical burner is used. In turbulent flames, the reduction in flame length of 30% compared to a circular burner is possible. In addition to a reduction of the burner length, a reduction of NO emissions will also result from the use of the elliptical burners, but CO production will increase.

#### 7.4: Recommendations for Further Study

There are several avenues for further study.

Further studies of the mechanism of splitting for the 4:1 AR elliptical burner and for the apparent axis switching of the laminar 3:1 AR elliptical burner are warranted.

One of the conclusions of this study is that that 4:1 AR elliptical burner has greater stability than the 3:1 AR elliptical burner due to a pool of OH radicals located between the split flame. It may be beneficial to conduct a survey of the radical concentration distribution conditions of the elliptical burners at conditions approaching the blowout velocity in order to support this statement.

It would be of benefit to study the acoustic properties of premixed flames from elliptical burners. In practical combustors, acoustic noise can create standing waves in the combustor which can negatively impact the combustor performance.

Finally, one of the difficulties in designing ULC burners is that they are subject to flame oscillations and frequent blowouts. This behavior is often driven by variation in inlet equivalence ratio, pressure, or velocity. It is possible that the enhanced turbulence and velocity decay of the 4:1 AR elliptical burner may mitigate some of the variations. It would be informative to perform a study to see how the elliptical burners behave with such fluctuations.

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## APPENDIX A: SAMPLE CALCULATIONS

Molecular Weight of Fuel:

$$MW_{fuel} = \frac{1}{\sum \frac{Y_i}{MW_i}} = \frac{1}{\frac{0.6}{44.068} + \frac{0.4}{2}} = 4.681$$

(40%  $H_2$  by mass in propane)

Stochiometric Equation:

$$aC H_8 + bH_2 + \left(\frac{10a+b}{2}\right)O_2 + 3.76\left(\frac{10a+b}{2}\right)N_2 = 3aCO_2 + \frac{8a+2b}{2}H_2O + 3.76\left(\frac{10a+b}{2}\right)N_2$$

For 40%  $H_2$  by mass:

$$a = 0.6 \left(\frac{4.681}{44}\right) = 0.0638$$
  $b = 0.4 \left(\frac{4.681}{2}\right) = 0.936$ 

Stoichiometric Air-Fuel Ratio:

$$\left(\frac{A}{F}\right)_{Stoich.} = \frac{\dot{m}_{air}}{\dot{m}_{C_3H_8} + \dot{m}_{H_2}} = \frac{Q_{air}MW_{air}}{Q_{C_3H_8}MW_{C_3H_8} + Q_{H_2}MW_{H_2}} = \frac{4.76\left(\frac{10a+b}{2}\right)28.8}{a(44) + b(2)} = 23.06$$

Jet exit velocity of burner:

$$0.4 = \frac{Q_{H_2}MW_{H_2}}{Q_{C_3H_8}MW_{C_3H_8} + Q_{H_2}MW_{H_2}} \Longrightarrow Q_{C_3H_8} = 0.4^{-1} \left(\frac{0.6Q_{H_2}MW_{H_2}}{MW_{C_3H_8}}\right) = 0.0682Q_{H_2}$$

$$\Phi = \frac{\left(\frac{A}{F}\right)_{\text{Stoich.}}}{\left(\frac{A}{F}\right)_{\text{Actual}}} \Longrightarrow \left(\frac{A}{F}\right)_{\text{Actual}} = \frac{\left(\frac{A}{F}\right)_{\text{Stoich.}}}{\Phi} = \frac{Q_{\text{air}}MW_{\text{air}}}{Q_{C_{3}H_{8}}MW_{C_{3}H_{8}} + Q_{H_{2}}MW_{H_{2}}}$$

 $= \frac{Q_{air} M W_{air}}{Q_{C_{3}H_{8}} \left( M W_{C_{3}H_{8}} + 14.69 M W_{H_{2}} \right)}$ 

$$Q_{air} = 2.547 \Phi Q_{C_3 H_8}$$

For V = 60 m/s, an elliptical burner of major diameter of 1 mm and minor diameter of 4 mm, and an equivalence ratio of 2.0

$$A_{burner} = \pi ab = \pi (0.0005)(0.002) = 3.142 \times 10^{-6} m^2$$

$$V_{jet} = \frac{Q_{Total}}{A_{burner}} \Rightarrow Q_{Total} = 60 \times 3.142 \times 10^{-6} = 0.000189 \frac{m^3}{s}$$

$$Q_{Total} = Q_{Air} + Q_{C_3H_8} + Q_{H_2} = 29.41 Q_{C_3H_8} + Q_{C_3H_8} + 14.69 Q_{C_3H_8}$$

$$Q_{C_3H_8} = 4.19 \times 10^{-6} \frac{m^3}{s}$$

$$Q_{C_{3}H_{8}} = 0.251 \frac{l}{\min}$$
  $Q_{H_{2}} = 3.68 \frac{l}{\min}$   $Q_{air} = 7.37 \frac{l}{\min}$ 

Emission Index Calculation:

$$EI_{i} = \frac{\chi_{i}}{\chi_{CO} + \chi_{CO_{2}}} \frac{xMW_{i}}{MW_{fuel}}$$

Given that

$$MW_{CO} = 28$$
  $MW_{CO2} = 44$   $MW_{NO} = 44$   $MW_{fuel} = 4.681$ 

Concentration of CO = 16.7 ppmConcentration of NO = 2.94 ppm Concentration of  $CO_2 = 0.4\%$ Concentration of  $O_2 = 18.4\%$ 

$$\chi_{CO} = \frac{16.7}{1000000} = 0.0000167 \qquad \qquad \chi_{CO_2} = \frac{0.4}{100} = 0.004$$
$$\chi_{NO} = \frac{2.94}{1000000} = 0.00000294$$

$$x = \chi_{C_3H_8}(\#C) = 0.0638(3) = 0.1914$$

$$EI_{CO} = \frac{\chi_i}{\chi_{CO} + \chi_{CO_2}} \frac{xMW_{CO}}{MW_{fuel}} = \frac{0.0000167}{0.0000167 + 0.004} \frac{0.1914(28)}{4.681} = 0.00476 \frac{kg_{CO}}{kg_{fuel}} = 4.76 \frac{g_{CO}}{kg_{fuel}}$$

# Reynolds Number Calculation:

Mixture averaged viscosity:

$$\mu_{mixture} = \sum_{i=1}^{n} \left( \frac{\chi_i \mu_i}{\sum_{j=1}^{n} \chi_j \phi_{ij}} \right)$$

where 
$$\phi_{ij} = \frac{1}{\sqrt{8}} \left( 1 + \frac{MW_i}{MW_j} \right)^{-\frac{1}{2}} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{\frac{1}{2}} \left( \frac{MW_j}{MW_i} \right)^{\frac{1}{4}} \right]^2$$

	Propane	Hydrogen	Air
MW	44.069	2	28.97112
Density			
(kg/m <sup>3</sup> )	1.7666466	0.080176	1.1614
μ	8.256E-06	9.00E-06	1.85E-05

$\pmb{\phi}_{ij}$		i		
		Propane	Hydrogen	Air
j	Propane	1	3.679648	1.944037
	Hydrogen	0.153193021	1	0.270175
	Air	0.571588323	1.908054	1

For a 40% by mass  $H_2$  in propane mixture of equivalence ratio of 1.0 at 20 m/s

$$\chi_{C_3H_8} = 0.013676852 \quad \chi_{H_2} = 0.209503 \quad \chi_{air} = 0.77682$$

$$\mu_{\text{mixture}} = \sum_{i=1}^{n} \frac{\chi_{C_{3}H_{8}} \mu_{i}}{\sum_{j=1}^{n} \chi_{j} \phi_{ij}} = \frac{\chi_{C_{3}H_{8}} \mu_{C_{3}H_{8}}}{\chi_{C_{3}H_{8}} \phi_{C_{3}H_{8}} + \chi_{H_{2}} \phi_{C_{3}H_{8},H_{2}} + \chi_{air} \phi_{C_{3}H_{8,air}}} + \frac{\chi_{H_{2}} \mu_{H_{2}}}{\chi_{H_{2}} \mu_{H_{2}}} + \frac{\chi_{air} \mu_{air}}{\chi_{air} \mu_{air}}$$

 $\frac{1}{\chi_{C_{3}H_{8}}\varphi_{H_{2},C_{3}H_{8}}+\chi_{H_{2}}\varphi_{H_{2},H_{2}}+\chi_{air}\varphi_{H_{2},air}}+\frac{1}{\chi_{C_{3}H_{8}}\varphi_{air,C_{3}H_{8}}+\chi_{H_{2}}\varphi_{air,H_{2}}+\chi_{air}\varphi_{air,air}}$ 

= 1.79872E - 05 Ns/m<sup>2</sup>  

$$\rho_{mixture} = \sum_{i=1}^{n} \chi_{i} \rho_{i} = \chi_{C_{3}H_{8}} \rho_{C_{3}H_{8}} + \chi_{H_{2}} \rho_{H_{2}} + \chi_{air} \rho_{air} = 0.943157864 \text{ kg/m}^{3}$$
$$\operatorname{Re} = \frac{\rho VD}{\mu} = \frac{0.943 * 20 * 0.002}{1.799E - 05} = 2098$$

Rayleigh Scattering Calculation:

$$I_{s} = C_{opt} I \Omega I_{seg} \frac{P_{gas} A_{o}}{R_{gas} T_{gas}} \left(\frac{d\sigma}{d\Omega}\right)_{eff} = \frac{KI}{T_{gas}} \left(\frac{d\sigma}{d\Omega}\right)_{eff}$$

$$K = \frac{I_{s,300} T_{300}}{I_{300} \left(\frac{d\sigma}{d\Omega}\right)_{eff}}$$

 $I_{s,300} = 2.89 \text{E} + 06 \text{ counts}$ 

$$T_{300} = 300 \text{ K}$$

 $I_{300} = 0.246 \text{ J}$ 

$$\left(\frac{d\sigma}{d\Omega}\right)_{eff} = \left(\frac{d\sigma}{d\Omega}\right)_{N_2} = 1.51504\text{E-}27 \text{ m}^2$$

$$K = \frac{2.89E + 06 \times 300}{0.246(1.51504E - 27)} = 2.326e36 \frac{counts \times K}{J \times m^2}$$

$$T_{gas} = \frac{KI}{I_s} \left(\frac{d\sigma}{d\Omega}\right)_{eff}$$

 $I_s = 9.43 \text{E} + 05 \text{ counts}$ 

*I* =0.252 J

$$T_{gas} = \frac{2.326e36*0.252}{9.43e05} 1.51504\text{E} - 27 = 941 \text{ K}$$
  
OH Fluorescent Calculation:

$$n_{pe} = C_{exp} \times n_A \times C_{SV}$$

$$n_A = \frac{I_L}{hv_{ge}} n_{OH} \beta_{ge} \sigma_{ge} \Delta l$$

$$I_L = 850 \ \mu J$$

$$h = 6.63E-34 \ J/s$$

$$v_{ge} = 1051524.711 \ s^{-1}$$

$$\beta_{ge} = 2.30E-02$$

$$\sigma_{ge} = 4.47E-22 \ m^2$$

$$\Delta l = 0.5 \ mm$$

$$n_{OH} = \frac{hv_{ge}}{I_L \beta_{ge} \sigma_{ge} \Delta l} n_A = \frac{6.63 \text{E} \cdot 34 * 1051524.711}{850 \text{ e} \cdot 6 * 2.30 \text{E} \cdot 02 * 4.47 \text{E} \cdot 22 * 0.0005} n_A = 159.6 * n_A$$
$$C_{\text{SV}} = \frac{A_{21}}{A_{21} + Q_{\text{C}}}$$

$$C_{\rm exp} = \left(\frac{\Omega}{4\pi}\eta_T\eta_D\right)$$

 $\Omega$  =0.003267111 steradians  $\eta_{\rm T}$  =0.1248  $\eta_{\rm D}$  =0.13

$$C_{exp} = \left(\frac{0.003267111}{4\pi} 0.1248 \times 0.13\right) = 3.667e - 6$$
  

$$C_{SV} = \frac{A_{21}}{A_{21} + Q_C}$$
  

$$A_{21} = 4.75E + 05 \text{ s}^{-1}$$
  

$$Q_C = \sum_{i} n_i q_{ix}$$
  

$$q_{ix} = a_i \sigma_q T^{0.5}$$

$$\sigma_q = \sigma_{Q_{\infty}} \exp\left(\frac{\varepsilon}{kT}\right)$$

Given the following number densities

 CO2
 CO
 H2O
 N2
 O2
 H2

 2.07439E+11
 0
 1.4817E+12
 3.971E+12
 0
 0
 0

a temperature of 2000 K, and Table 3.3:

$$\sigma_{CO_2} = 11 \exp\left(\frac{624}{2000}\right) = 14.04 \qquad q_{ix} = 4.16e^{-13} 14.04(2000)^{0.5} = 2.61e \cdot 10$$
  
$$\sigma_{H_2O} = 20 \exp\left(\frac{434}{2000}\right) = 24.8 \qquad q_{ix} = 4.92e^{-13} 24.8(2000)^{0.5} = 5.46e \cdot 10$$
  
$$\sigma_{N_2} = 0.4 \exp\left(\frac{624}{2000}\right) = 0.5464 \qquad q_{ix} = 4.47e^{-13} 0.546(2000)^{0.5} = 1.092e \cdot 11$$

$$Q_{c} = 2.07e11 \times 2.61e - 10 + 1.48e12 \times 5.46e - 10 + 3.97e12 \times 1.092e - 11 = 907614455$$

$$C_{SV} = \frac{475000}{475000 + 907614455} = 0.00523$$

Rearranging

$$n_{pe} = \frac{DetectorCount}{CountsperPhotoelectron \times number of shots} = \frac{474975.5}{100.48*300} = 15.76$$

$$n_a = \frac{n_{pe}}{C_{\exp} \times C_{SV}} = \frac{15.76}{3.667e - 6 \times 0.00523} = 8.216e8$$

 $n_{OH} = 159.55 * 8.216e8 = 1.3e11$ 

# **APPENDIX B: UNCERTAINTY CALCULATION**

Sample calculation of uncertainty Given the following

NO
(ppm)
69.6
68.9
70.9
80.7
82.6
73.5
78.4
76.9
73.5
69.2

Average NO = 74.42Standard Deviation = 4.982

Standard Deviation of the mean  $=\frac{\sigma}{\sqrt{n}}=\frac{4.982}{\sqrt{10}}=1.575$ 

For a confidence interval of 95%, using the Students t test:

$$t_{\alpha/2} = 2.262159$$

$$\omega_{NO} = t_{\alpha/2} \times \sigma_{mean} = 3.56$$

Thus NO =  $74.42 \pm 3.56$  ppm.

#### **APPENDIX C: THEORY BEHIND FLUENT CALCULATIONS**

The following is adapted from Fluent.Inc (2001).

## **C.1: Continuity and Momentum**

## C.1.1 Instantaneous Navier-Stokes Equations:

In this section, the conservation equations for laminar flow will presented. The conservation equations relevant to heat transfer, turbulence modeling, and species transport will be discussed in subsequent sections.

**C.1.1.1 The Mass Conservation Equation:** The equation for conservation of mass, or continuity equation, is written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \tag{C.1.1}$$

where a source  $S_m$  is the mass added to the system i.e., due to evaporation of a liquid, ablation of a solid surface, etc.

For 2D axisymmetric geometries, the continuity equation can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial r}(\rho v_r) + \frac{\rho v_r}{r} = S_m$$
C.1.2

where x is the axial coordinate, r is the radial coordinate,  $v_x$  is the axial velocity, and  $v_r$  is the radial velocity.

**C.1.1.2 Momentum Conservation Equations**: Conservation of momentum for laminar flow in is described by

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\overline{\tau}) + \rho \vec{g} + \vec{F}$$
C.1.3

where p is the static pressure,  $\overline{\overline{\tau}}$  is the stress tensor (described below), and  $\vec{pg}$  and  $\vec{F}$ 

are the gravitational body force and external body forces respectively.  $\vec{F}$  can also contain other model-dependent source terms such as porous-media and user-defined sources.

The stress tensor  $\overline{\overline{\tau}}$  is given by

$$\overline{\overline{\tau}} = \mu \left[ (\nabla \vec{v} + \nabla \vec{v}^{\mathrm{T}}) - \frac{2}{3} \nabla \cdot \vec{v} I \right]$$
C.1.4

where  $\mu$  is the molecular viscosity, *I* is the unit tensor, and the second term on the right hand side is the effect of volume dilation.

## C.1.1.3 Convective Heat and Mass Transfer Modeling

The heat transfer in the system is given as:

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}[u_i(\rho E + p)] = \frac{\partial}{\partial x_j} \left[ \left(k + \frac{c_p \mu_t}{\Pr_t}\right) \frac{\partial T}{\partial x_j} + u_i(\tau_{ij})_{\text{eff}} \right] + S_h \quad \text{C.1.5}$$

where E is the total energy  $(\tau_{ij})_{eff}$  and is the deviatoric stress tensor, defined as

$$(\tau_{ij})_{\text{eff}} = \mu_{\text{eff}} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{2}{3} \mu_{\text{eff}} \frac{\partial u_i}{\partial x_i} \delta_{ij}$$
C.1.6

The term involving  $(\tau_{ij})_{\text{eff}}$  represents the viscous heating.

Turbulent mass transfer is treated similarly, with a default turbulent Schmidt number of 0.7.

### C.1.2 Reynolds (Ensemble) Averaging:

In Reynolds averaging, the solution variables in the instantaneous (exact) Navier-Stokes equations are decomposed into the mean (ensemble-averaged or time-averaged) and fluctuating components. For the velocity components:

$$u_i = \bar{u}_i + u'_i \tag{C.1.7}$$

where  $\bar{u}_i$  and  $u'_i$  are the mean and fluctuating velocity components (i = 1, 2, 3).

Likewise, for pressure and other scalar quantities:

$$\phi = \bar{\phi} + \phi' \tag{C.1.8}$$

where  $\phi$  denotes a scalar such as pressure, energy, or species concentration.

Substituting expressions of this form for the flow variables into the instantaneous continuity and momentum equations and taking a time (or ensemble) average (and dropping the overbar on the mean velocity,  $\mathbf{\bar{u}}$ ) yields the ensemble-averaged momentum equations. They can be written in Cartesian tensor form as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0 \qquad C.1.9$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] + \frac{\partial}{\partial x_j} (-\rho \overline{u'_i u'_j}) \qquad C.1.10$$

Equations C.1.3 and C.1.4 are called Reynolds-averaged Navier-Stokes (RANS) equations. They have the same general form as the instantaneous Navier-Stokes equations, with the velocities and other solution variables now representing ensemble-

averaged (or time-averaged) values. Additional terms now appear that represent the effects of turbulence. These Reynolds stresses,  $-\rho \overline{u'_i u'_j}$ , must be modeled in order to close Equation C.1.10.

For variable-density flows, Equations C.1.9 and C.1.10 can be interpreted as Favre-averaged Navier-Stokes equations, with the velocities representing mass-averaged values. As such, they can be applied to density-varying flows.

## **C.2 Turbulence Modeling:**

The turbulence model for Fluent was modeled using a Reynolds Stress Model (RSM).

## **C.2.1 Transport Equations for Reynolds Stresses:**

In this model, the transport equations for the transport of the Reynolds stresses, are given by

$$\frac{\partial}{\partial t}(\rho \ \overline{u'_i u'_j}) + \frac{\partial}{\partial x_k}(\rho u_k \overline{u'_i u'_j}) =$$

Local Time Derivative  $C_{ij} \equiv \text{Convection}$ 

$$\underbrace{-\frac{\partial}{\partial x_k} \left[ \rho \,\overline{u'_i u'_j u'_k} + \overline{p \left( \delta_{kj} u'_i + \delta_{ik} u'_j \right)} \right]}_{D_{T,ij} \equiv \text{ Turbulent Diffusion}} + \underbrace{\frac{\partial}{\partial x_k} \left[ \mu \frac{\partial}{\partial x_k} (\overline{u'_i u'_j}) \right]}_{D_{L,ij} \equiv \text{ Molecular Diffusion}}$$

$$\underbrace{-\rho\left(\overline{u_i'u_k'} \frac{\partial u_j}{\partial x_k} + \overline{u_j'u_k'} \frac{\partial u_i}{\partial x_k}\right)}_{P_{ij} \equiv \text{Stress Production}} G_{ij} \underbrace{-\rho\beta(g_i\overline{u_j'\theta} + g_j\overline{u_i'\theta})}_{\text{Buoyancy Production}}$$

$$+ \underbrace{p\left(\frac{\partial u'_{i}}{\partial x_{j}} + \frac{\partial u'_{j}}{\partial x_{i}}\right)}_{\phi_{ij} \equiv \text{ Pressure Strain } \epsilon_{ij} \equiv \text{ Dissipation}} - \underbrace{2\mu \frac{\partial u'_{i}}{\partial x_{k}} \frac{\partial u'_{j}}{\partial x_{k}}}_{ij \equiv \text{ Dissipation}} + \underbrace{-2\rho \Omega_{k} \left(\overline{u'_{j}u'_{m}}\epsilon_{ikm} + \overline{u'_{i}u'_{m}}\epsilon_{jkm}\right)}_{F_{ij} \equiv \text{ Production by System Rotation}} + \underbrace{S_{user}}_{User-Defined Source Term} C.2.1$$

The  $C_{ij}$ ,  $D_{L,ij}$ ,  $P_{ij}$ , and  $F_{ij}$  terms are exact. However, in order to solve the system,  $D_{T,ij}$ ,  $G_{ij}$ ,  $\phi_{ij}$ , and  $\varepsilon_{ij}$  need to be appropriately modeled.

**C.2.1.1 Turbulent Diffusion Model:** *D*<sub>*T*,*ij*</sub> can be modeled by:

$$D_{T,ij} = \frac{\partial}{\partial x_k} \left( \frac{\mu_t}{\sigma_k} \frac{\partial \overline{u'_i u'_j}}{\partial x_k} \right)$$
C.2.2

The turbulent viscosity, *µ*, is computed using

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon}$$
 C.2.3

where  $C_{\mu}=0.09$  .

and  $\sigma_k=0.82$ 

C.2.1.2 Pressure-Strain Term Model: In FLUENT, the pressure-strain term, in Equation C.2.1 is modeled by

$$\phi_{ij} = \phi_{ij,1} + \phi_{ij,2} + \phi_{ij,w} \tag{C.2.4}$$

The slow pressure-  $\phi_{ij,1}$  strain term, , is modeled as

$$\phi_{ij,1} \equiv -C_1 \rho \, \frac{\epsilon}{k} \left[ \overline{u'_i u'_j} - \frac{2}{3} \delta_{ij} k \right]$$
C.2.5

with  $C_1 = 1.8$ .

The rapid pressure-strain term,  $\phi_{ij,2}$  , is modeled as

$$\phi_{ij,2} \equiv -C_2 \left[ (P_{ij} + F_{ij} + G_{ij} - C_{ij}) - \frac{2}{3} \delta_{ij} (P + G - C) \right]$$
C.2.6

where  $C_2 = 0.60$ ,  $P_{ij}$ ,  $F_{ij}$ ,  $G_{ij}$ , and  $C_{ij}$  are the same as what is given in Equation C.2.1,

$$P=rac{1}{2}P_{kk}$$
 ,  $G=rac{1}{2}G_{kk}$  , and  $C=rac{1}{2}C_{kk}$ 

The wall-reflection term,  $\phi_{ij,w}$ , is modeled as

$$\begin{split} \phi_{ij,w} &\equiv C_{1}' \frac{\epsilon}{k} \left( \overline{u_{k}' u_{m}'} n_{k} n_{m} \delta_{ij} - \frac{3}{2} \overline{u_{i}' u_{k}'} n_{j} n_{k} - \frac{3}{2} \overline{u_{j}' u_{k}'} n_{i} n_{k} \right) \frac{k^{3/2}}{C_{\ell} \epsilon d} \\ &+ C_{2}' \left( \phi_{km,2} n_{k} n_{m} \delta_{ij} - \frac{3}{2} \phi_{ik,2} n_{j} n_{k} - \frac{3}{2} \phi_{jk,2} n_{i} n_{k} \right) \frac{k^{3/2}}{C_{\ell} \epsilon d} \end{split}$$

where  $C_1 = 0.5$ ,  $C_2 = 0.3$ ,  $n_k$  is the  $x_k$  component of the unit normal to the wall, d is the normal distance to the wall, and  $C_{\ell} = C_{\mu}^{3/4} / \kappa$ , where  $C_{\mu} = 0.09$  and  $\kappa$  is the von Kármán constant (= 0.4187).

**C.2.1.3 Buoyancy Effects on Turbulence:** The production terms due to buoyancy are modeled as

$$G_{ij} = \beta \frac{\mu_t}{\Pr_t} \left( g_i \frac{\partial T}{\partial x_j} + g_j \frac{\partial T}{\partial x_i} \right)$$
C.2.8

where  $Pr_t$  is the turbulent Prandtl number for energy, with a default value of 0.85.

 $G_{ij}$  is calculated by

$$G_{ij} = -rac{\mu_t}{
ho \mathrm{Pr}_t} \left( g_i rac{\partial 
ho}{\partial x_j} + g_j rac{\partial 
ho}{\partial x_i} 
ight)$$

**C.2.1.4 Turbulence Kinetic Energy Model:** In general, when the turbulence kinetic energy is needed for modeling a specific term, it is obtained by taking the trace of the Reynolds stress tensor:

$$k = \frac{1}{2} \overline{u'_i u'_i}$$
C.2.9

C.2.1.5 Dissipation Rate Tensor Model: The dissipation tensor, 4 , is modeled by

$$\epsilon_{ij} = \frac{2}{3} \delta_{ij} (\rho \epsilon + Y_M) \tag{C.2.10}$$

where  $Y_M = 2\rho \epsilon M_t^2$  is an additional ``dilatation dissipation" term. Since the flow

modeled was incompressible, M<sub>t</sub> is equal to zero, therefore the "dilation dissipation" term neglected.

The scalar dissipation rate, €, for the dissipation tensor is computed by

$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial x_i}(\rho\epsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial\epsilon}{\partial x_j} \right] + C_{\epsilon 1} \frac{1}{2} \left[ P_{ii} + C_{\epsilon 3} G_{ii} \right] \frac{\epsilon}{k} - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} + S_{\epsilon}$$
C.2.11

where  $\sigma_{\epsilon} = 1.0$ ,  $C_{\epsilon 1} = 1.44$ ,  $C_{\epsilon 2} = 1.92$ ,  $C_{\epsilon 3}$  is evaluated as a function of the local flow direction relative to the gravitational vector and  $S_{\epsilon}$  is a user-defined source term.

## C.2.2 Boundary Conditions for the Reynolds Stresses:

Where the flow enters the computational domain, the boundary conditions for the individual Reynolds stresses,  $\overline{u'_i u'_j}$ , and for the turbulence dissipation rate,  $\epsilon$ , are derived from the turbulence intensity and characteristic length.

At walls in the domain, the near-wall values of the Reynolds stresses and  $\epsilon$  are calculated from wall functions. **FLUENT** applies explicit wall boundary conditions for the Reynolds stresses by using the log-law and the assumption of equilibrium, disregarding convection and diffusion in the transport equations for the stresses (Equation C.2.1). The Reynolds stresses at the wall-adjacent cells are computed from

$$\frac{\overline{u_{\tau}^{\prime 2}}}{k} = 1.098, \quad \frac{\overline{u_{\eta}^{\prime 2}}}{k} = 0.247, \quad \frac{\overline{u_{\lambda}^{\prime 2}}}{k} = 0.655, \quad -\frac{\overline{u_{\tau}^{\prime} u_{\eta}^{\prime}}}{k} = 0.255$$
(C.2.12)

where  $\tau$  is the tangential coordinate,  $\eta$  is the normal coordinate, and  $\lambda$  is the binormal coordinate. FLUENT solves the transport equation to obtain k.

## C.3 Reaction Modelling

## C.3.1 The Eddy-Dissipation Model:

For fast burning flames the overall rate of reaction is controlled by mixing due to turbulence. For non-premixed flames, turbulence has the effect of slowly mixing the fuel and oxidizer at the reaction zone. Combustion then proceeds quickly. The turbulence in premixed flames slowly mixes cold, unburned fuel/air mixture with the hot product gases. In such mixing limited cases, the combustion chemical kinetic rates can be neglected with the assumption that combustion rates are much faster than the rate at which mixing occurs.

One turbulence-chemistry interaction model provided by **FLUENT** is the eddydissipation model. For this model, the net rate of production of species *i* due to reaction *r*,  $R_{i,r}$ , is given by the smaller result of the following two expressions:

$$R_{i,r} = \nu_{i,r}' M_{w,i} A \rho \frac{\epsilon}{k} \min_{\mathcal{R}} \left( \frac{Y_{\mathcal{R}}}{\nu_{\mathcal{R},r}' M_{w,\mathcal{R}}} \right)$$
(C.3.1)

$$R_{i,r} = \nu'_{i,r} M_{w,i} A B \rho \frac{\epsilon}{k} \frac{\sum_P Y_P}{\sum_j^N \nu''_{j,r} M_{w,j}}$$
(C.3.2)

where  $Y_P$  is the mass fraction of any product species, P

 $Y_{\mathcal{R}}$  is the mass fraction of a particular reactant,  $\mathcal{R}$ 

- *A* is an empirical constant equal to 4.0
- *B* is an empirical constant equal to 0.5

In Equations C.3.1 and C.3.2, the chemical reaction rate is governed by the large-eddy mixing  $k/\epsilon$  time scale, . Combustion proceeds whenever turbulence is present, that is,  $k/\epsilon > 0$ , thus ignition source is not required for the initiation of combustion. This method works for non-premixed flames, but in premixed flames, however, this simplification causes the reactants to burn immediately as they enter the computational domain which is not physically correct. To correct for this, the net reaction rate is taken as the minimum of these two rates provided by an Arrhenius reaction rate formulation and the eddy dissipation model given by equations C.3.1 and C.3.2. The Arrhenius rate acts to prevent the development of the reaction zone until ignition would normally occur in the system. Once ignition occurs, the mixing limited combustion comes into effect. For this Arrhenius/eddy-dissipation model, the reaction kinetics models should be keep small (two or less steps) due to inability of the eddy-dissipation model to predict kinetically controlled species.

### C.3.2 The Eddy-Dissipation-Concept (EDC) Model:

An extension to the eddy-dissipation model which includes detailed chemical kinetics mechanisms in turbulent flows is the eddy-dissipation-concept (EDC) model.

The EDC model assumes that reaction occurs in small turbulent structures. The volume fraction of the small turbulent structures is modeled as

$$\boldsymbol{\xi}^* = C_{\boldsymbol{\xi}} \left(\frac{\nu\epsilon}{k^2}\right)^{3/4} \tag{C.3.3}$$

where \* denotes the small turbulent structure quantities and

$$C_{\epsilon}$$
 = volume fraction constant = 2.1377

 $\mathbf{v}$  = kinematic viscosity

Species are assumed to react in the turbulent structures over a time scale

$$\tau^* = C_\tau \left(\frac{\nu}{\epsilon}\right)^{1/2} \tag{C.3.4}$$

where  $C_{\tau}$  is a time scale constant equal to 0.4082.

In **FLUENT**, combustion in the small turbulent structures is assumed to occur as a constant pressure reactor. Initial conditions of this reactor are taken as cell's current species and temperature. Reactions then proceed over the time scale  $\tau^*$ , governed by the Arrhenius rates, and are integrated numerically with CVODE. The species state after reacting for a time  $\tau^*$  is denoted by  $Y_{i}^*$ .

The source term in the conservation equation for the mean species *i*, is modeled as

$$R_{i} = \frac{\rho(\xi^{*})^{2}}{\tau^{*}[1 - (\xi^{*})^{3}]} (Y_{i}^{*} - Y_{i})$$
(C.3.5)

#### **APPENDIX D: THEORY BEHIND CHEMKIN CALCULATIONS**

For the calculations simulating the freezing of the CO reactions in the flames, the Chemkin chemical reaction modeling package was used. The theory behind the Chemkin calculations is as follows (adapted from the Chemkin documentation (2003)).

## **D.1:** Governing Equations

The equations governing steady, isobaric, quasi-one-dimensional flame propagation are written as follows:

Continuity:

$$\dot{M} = \rho u A$$
 D.1.1

Energy:

$$\dot{M}\frac{dT}{dx} + \frac{1}{c_p}\frac{d}{dx}\left(\lambda A\frac{dT}{dx}\right) - \frac{A}{c_p}\sum_{k=1}^{K}\dot{\omega}_k h_k W_k = 0$$
D.1.2

Species:

$$\dot{M}\frac{dY_k}{dx} + \frac{d}{dx}(\rho AY_k V_k) - A\dot{\omega}_k W_k = 0$$
 D.1.3

Equation of State:

$$\rho = \frac{P\overline{W}}{RT}$$
D.1.4

In these equations x denotes the spatial coordinate;  $\dot{M}$  the mass flow rate (which is independent of x); T the temperature;  $Y_k$  the mass fraction of the kth species (there are  $K_g$  species); P the pressure; u the velocity of the fluid mixture;  $\rho$  the mass density;  $W_k$  the molecular weight of the kth species;  $\overline{W}$  the mean molecular weight of the mixture; *R* the universal gas constant;  $\lambda$  the thermal conductivity of the mixture;  $c_p$  the constant-pressure heat capacity of the mixture;  $c_{pk}$  the constant pressure heat capacity of the *k*th species;  $\dot{\omega}_k$  the molar rate of production by chemical reaction of the *k*th species per unit volume;  $h_k$  the specific enthalpy of the *k*th species;  $V_k$  the diffusion velocity of the *k*th species; and *A* the cross-sectional area of the stream tube encompassing the flame (normally increasing due to thermal expansion) normalized by the burner area.

#### **D.2:** Chemical Reaction Modeling

The net chemical production rate  $\dot{\omega}_k$  of each species results from the interaction of all the chemical reactions involving that species. Each reaction proceeds according to the law of mass action and the forward rate coefficients and is the reactions are described by the modified Arrhenius form,

$$k_f = AT^{\beta} \exp\left(\frac{-E_A}{RT}\right)$$
D.2.1

#### **D.3: Boundary Conditions**

Two different types of flames are modeled with the Chemkin PREMIX code: burner-stabilized flames and adiabatic, freely propagating flames. The flames are modeled with the same conservation equations but the boundary conditions differ for the two cases. Burner stabilized flames are modeled by having  $\dot{M}$  as a known constant, specifying the temperature and mass flux fractions  $\left(\varepsilon_{k} = Y_{k} + \rho Y_{k} \frac{A}{\dot{M}}\right)$  upstream of the flame by:

$$\varepsilon_{k,1} - Y_{k,1} - \left(\frac{\rho A Y_k V_k}{\dot{M}}\right)_{j=1/2} = 0$$
 D.4.1

and

where  $\varepsilon_{k,1}$  is the inlet reactant fraction of the *k*th species (see Keyword REAC) and  $T_b$  is a specified burner temperature. Downstream of the reaction zone, the boundary is set to a vanishing gradient:

$$\frac{Y_{k,J} - Y_{k,J-1}}{x_{k,J} - x_{k,J-1}} = 0$$
 D.4.3

and

For a freely propagating flame  $\dot{M}$  is not known beforehand and therefore must be determined as part of the solution. In addition to the boundary equations given above, an additional constraint is required. Fluent applies this constraint by setting the location of the flame. This is done by fixing the temperaturare at one point of the system.

Once these boundary conditions are applied Fluent solves the system.

#### **APPENDIX E: CHEMKIN MODEL FOR QIN, ET AL. (2000)**

**ELEMENTS** C H O N AR END SPECIES 02 OH H2O HO2 H2O2 H2 Н 0 CH2 CH2\* CH3 CH4 CO CO2 С CH НСО СН2О СН2ОН СН3О СН3ОН С2Н С2Н2 С2Н3 С2Н4 С2Н5 С2Н6 НССО СН2СО НССОН AR N2 СН2СНО СЗН2 СЗН3 рСЗН4 аСЗН4 сСЗН4 C4H2 H2C4O n-C4H3 i-C4H3 C4H4 n-C4H5 i-C4H5 C4H6 C4H612 C4H81 C4H7 C6H2 C6H3 1-C6H4 c-C6H4 A1 A1-C6H5O C6H5OH C5H6 C5H5 C5H5O C5H4OH C5H4O C3H8 nC3H7 iC3H7 C3H6 aC3H5 CH3CCH2 CH3CHO C2H3CHO **END** ! GRI-Mech Version 3.0 7/30/99 CHEMKIN-II format (C  $\leq$  3) and (Qin&Scott C3 & Scott C4-C6) REACTIONS 2O+M<=>O2+M 1.200E+17 -1.000 .00 H2/2.40/H2O/15.40/CH4/2.00/CO/1.75/CO2/3.60/C2H6/3.00/AR/.83/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ 5.000E+17 -1.000 O+H+M<=>OH+M .00 H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/  $O+H2 \leq H+OH$ 3.870E+04 2.700 6260.00 O+HO2<=>OH+O2 2.000E+13 .000 .00 O+H2O2<=>OH+HO2 9.630E+06 2.000 4000.00 O+CH<=>H+CO 5.700E+13 .000 .00 O+CH2<=>H+HCO 8.000E+13 .000 .00 O+CH2\*<=>H2+CO 1.500E+13 .000 .00 O+CH2\*<=>H+HCO .00 1.500E+13 .000 O+CH3<=>H+CH2O 5.060E+13 .000 .00 O+CH4<=>OH+CH3 1.020E+09 1.500 8600.00 1.800E+10 .000 2385.00  $O+CO(+M) \leq >CO2(+M)$ LOW/ 6.020E+14 .000 3000.00/ H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ O+HCO<=>OH+CO 3.000E+13 .000 .00 .000 O+HCO<=>H+CO2 3.000E+13 .00 O+CH2O<=>OH+HCO 3.900E+13 .000 3540.00 O+CH2OH<=>OH+CH2O 1.000E+13 .000 .00 O+CH3O<=>OH+CH2O 1.000E+13 .000 .00 3.880E+05 2.500 3100.00 O+CH3OH<=>OH+CH2OH O+CH3OH<=>OH+CH3O 1.300E+05 2.500 5000.00 O+C2H<=>CH+CO 5.000E+13 .000 .00 O+C2H2<=>H+HCCO 1.350E+07 2.000 1900.00  $O+C2H2 \le OH+C2H$ 4.600E+19 -1.410 28950.00 O+C2H2<=>CO+CH2 6.940E+06 2.000 1900.00 O+C2H3<=>H+CH2CO 3.000E+13 .000 .00 O+C2H4<=>CH3+HCO 2.500E+07 1.830 220.00 ! k\_opt=2\*ko

O+C2H5<=>CH3+CH2O 2.240E+13 .000 .00 O+C2H6<=>OH+C2H5 8.980E+07 1.920 5690.00 O+HCCO<=>H+2CO 1.000E+14 .000 .00 O+CH2CO<=>OH+HCCO 1.000E+13 .000 8000.00 O+CH2CO<=>CH2+CO2 1.750E+12 .000 1350.00  $O2+CO \le O+CO2$ 2.500E+12 .000 47800.00 O2+CH2O<=>HO2+HCO 1.000E+14 .000 40000.00  $H+O2+M \le HO2+M$ 2.800E+18 -.860 00 O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/ AR/ .00/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ H+2O2<=>HO2+O2 2.080E+19 -1.240 .00 H+O2+H2O<=>HO2+H2O 11.26E+18 -.760 .00 2.600E+19 -1.240 .00  $H+O2+N2 \le HO2+N2$ 7.000E+17 -.800  $H+O2+AR \le HO2+AR$ .00 2.650E+16 -.6707 17041.00 H+O2<=>O+OH  $2H+M \le H2+M$ 1.000E+18 -1.000.00 H2/.00/H2O/.00/CH4/2.00/CO2/.00/C2H6/3.00/AR/.63/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ 2H+H2<=>2H2 9.000E+16 -.600 .00 2H+H2O<=>H2+H2O 6.000E+19 -1.250 .00 2H+CO2<=>H2+CO2 5.500E+20 -2.000 .00  $H+OH+M \le H2O+M$ 2.200E+22 -2.000 .00 H2/.73/H2O/3.65/CH4/2.00/C2H6/3.00/AR/.38/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/  $H+HO2 \le O+H2O$ .000 671.00 3.970E+12 7.750E+13 H+HO2<=>O2+H2 .000 1068.00 ! k opt=1.73\*ko H+HO2<=>2OH 0.420E+14 .000 635.00 ! k opt=0.5\*ko H+H2O2<=>HO2+H2 1.210E+07 2.000 5200.00  $H+H2O2 \le OH+H2O$ 1.000E+13 .000 3600.00 .000  $H+CH \le C+H2$ 1.650E+14 .00 6.000E+14 .000  $H+CH2(+M) \leq >CH3(+M)$ .00 LOW / 1.040E+26 -2.760 1600.00/ TROE/ .5620 91.00 5836.00 8552.00/ H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ H+CH2\*<=>CH+H2 3.000E+13 .000 .00  $H+CH3(+M) \leq >CH4(+M)$ 13.90E+15 -.534 536.00 LOW / 2.620E+33 -4.760 2440.00/ TROE/ .7830 74.00 2941.00 6964.00 / H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ H+CH4<=>CH3+H2 6.600E+08 1.620 10840.00  $H+HCO(+M) \leq >CH2O(+M)$ 1.090E+12 .480 -260.00 LOW / 2.470E+24 -2.570 425.00/ TROE/ .7824 271.00 2755.00 6570.00 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ H+HCO<=>H2+CO 7.340E+13 .000 .00  $H+CH2O(+M) \leq CH2OH(+M)$ 5.400E+11 .454 3600.00 LOW / 1.270E+32 -4.820 6530.00/ TROE/ .7187 103.00 1291.00 4160.00 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/  $H+CH2O(+M) \leq >CH3O(+M)$ 5.400E+11 .454 2600.00 LOW / 2.200E+30 -4.800 5560.00/ TROE/ .7580 94.00 1555.00 4200.00 /

```
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
H+CH2O<=>HCO+H2
                                5.740E+07 1.900 2742.00
H+CH2OH(+M) \leq >CH3OH(+M)
                                      1.055E+12 .500
                                                        86.00
  LOW / 4.360E+31 -4.650 5080.00/
  TROE/ .600 100.00 90000.0 10000.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
H+CH2OH<=>H2+CH2O
                                  2.000E+13
                                             .000
                                                     .00
H+CH2OH<=>OH+CH3
                                  1.650E+11
                                            .650 -284.00
H+CH2OH<=>CH2*+H2O
                                 3.280E+13 -.090 610.00
H+CH3O(+M) \leq CH3OH(+M)
                                     2.430E+12 .515
                                                       50.00
  LOW / 4.660E+41 -7.440 14080.0/
  TROE/ .700 100.00 90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
H+CH3O<=>H+CH2OH
                                 4.150E+07 1.630 1924.00
H+CH3O \leq H2+CH2O
                                 2.000E+13
                                             .000
                                                    .00
H+CH3O<=>OH+CH3
                                1.500E+12
                                            .500 -110.00
H+CH3O<=>CH2*+H2O
                                2.620E+14 -.230 1070.00
                                   1.700E+07 2.100 4870.00
H+CH3OH<=>CH2OH+H2
H+CH3OH<=>CH3O+H2
                                  4.200E+06 2.100 4870.00
H+C2H(+M) \leq >C2H2(+M)
                                  1.000E+17 -1.000
                                                      .00
  LOW / 3.750E+33 -4.800 1900.00/
  TROE/ .6464 132.00 1315.00 5566.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
H+C2H2(+M) \le C2H3(+M)
                                             .000 2400.00
                                   5.600E+12
  LOW / 3.800E+40 -7.270 7220.00/
  TROE/ .7507 98.50 1302.00 4167.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
H+C2H3(+M) \le C2H4(+M)
                                  6.080E+12 .270
                                                    280.00
  LOW / 1.400E+30 -3.860 3320.00/
  TROE/ .7820 207.50 2663.00 6095.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
                                3.030E+13 .000
H+C2H3<=>H2+C2H2
                                                    .00 ! k opt=1.01*ko
H+C2H4(+M) \le C2H5(+M)
                                   0.783E+12 .454 1820.00 ! k opt=1.45*ko
  LOW / 0.600E+42 -7.620 6970.00/
  TROE/ .9753 210.00 984.00 4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
H+C2H4<=>C2H3+H2
                                1.325E+06 2.530 12240.00
H+C2H5(+M) \le C2H6(+M)
                                   5.210E+17 -.990 1580.00
  LOW / 1.990E+41 -7.080 6685.00/
  TROE/ .8422 125.00 2219.00 6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
H+C2H5 <=>H2+C2H4
                                2.000E+12
                                            .000
                                                    .00
                                1.150E+08 1.900
H+C2H6 \le C2H5+H2
                                                  7530.00
H+HCCO<=>CH2*+CO
                                1.000E+14
                                           .000
                                                    00
H+CH2CO<=>HCCO+H2
                                  5.000E+13
                                              .000 8000.00
                                 1.130E+13
H+CH2CO<=>CH3+CO
                                             .000
                                                  3428.00
                                  1.000E+13
                                              .000
H+HCCOH<=>H+CH2CO
                                                      .00
H2+CO(+M) \leq CH2O(+M)
                                  4.300E+07 1.500 79600.00
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LOW / 5.070E+27 -3.420 84350.00/ TROE/ .9320 197.00 1540.00 10300.00 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/  $OH+H2 \leq H+H2O$ 2.160E+08 1.510 3430.00  $2OH(+M) \le H2O2(+M)$ 7.400E+13 -.370 .00 LOW / 2.300E+18 -.900 -1700.00/ TROE/ .7346 94.00 1756.00 5182.00 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ 20H<=>O+H2O 3.570E+04 2.400 -2110.00 OH+HO2<=>O2+H2O 1.450E+13 .000 -500.00 DUPLICATE OH+H2O2<=>HO2+H2O 2.000E+12 .000 427.00 DUPLICATE OH+H2O2<=>HO2+H2O 1.700E+18 .000 29410.00 DUPLICATE 5.000E+13 .000 OH+C<=>H+CO .00 OH+CH<=>H+HCO 3.000E+13 .000 .00 OH+CH2<=>H+CH2O 2.000E+13 .000 .00 OH+CH2<=>CH+H2O 1.130E+07 2.000 3000.00 OH+CH2\*<=>H+CH2O 3.000E+13 .000 .00  $OH+CH3(+M) \leq CH3OH(+M)$ 2.790E+18 -1.430 1330.00 LOW / 4.000E+36 -5.920 3140.00/ TROE/ .4120 195.0 5900.00 6394.00/ H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/  $OH+CH3 \leq >CH2+H2O$ 5.600E+07 1.600 5420.00  $OH+CH3 \leq >CH2*+H2O$ 6.440E+17 -1.340 1417.00 1.000E+08 1.600 3120.00 OH+CH4<=>CH3+H2O  $OH+CO \le H+CO2$ 4.760E+07 1.228 70.00 OH+HCO<=>H2O+CO 5.000E+13 .000 .00 OH+CH2O<=>HCO+H2O 3.430E+09 1.180 -447.00 OH+CH2OH<=>H2O+CH2O 5.000E+12 .000 .00 OH+CH3O<=>H2O+CH2O 5.000E+12 .000 .00 OH+CH3OH<=>CH2OH+H2O 1.440E+06 2.000 -840.00 OH+CH3OH<=>CH3O+H2O 6.300E+06 2.000 1500.00 2.000E+13 .000 OH+C2H<=>H+HCCO .00 OH+C2H2<=>H+CH2CO 2.180E-04 4.500 -1000.00 5.040E+05 2.300 13500.00 OH+C2H2<=>H+HCCOH OH+C2H2<=>C2H+H2O 3.370E+07 2.000 14000.00 OH+C2H2<=>CH3+CO 4.830E-04 4.000 -2000.00 OH+C2H3<=>H2O+C2H2 5.000E+12 .000 .00 1.800E+06 2.000 2500.00 ! k opt=0.5\*ko OH+C2H4<=>C2H3+H2O OH+C2H6<=>C2H5+H2O 3.540E+06 2.120 870.00 OH+CH2CO<=>HCCO+H2O 7.500E+12 .000 2000.00 2HO2<=>O2+H2O2 1.300E+11 .000 -1630.00 DUPLICATE 2HO2<=>O2+H2O2 4.200E+14 .000 12000.00 DUPLICATE HO2+CH2<=>OH+CH2O 2.000E+13 .000 .00 .00 HO2+CH3<=>O2+CH4 1.000E+12 .000 HO2+CH3<=>OH+CH3O 2.870E+13 .000 .00 ! k opt=0.76\*ko HO2+CO<=>OH+CO2 .000 23600.00 1.500E+14 HO2+CH2O<=>HCO+H2O2 5.600E+06 2.000 12000.00 C+O2<=>O+CO 5.800E+13 .000 576.00

 $C+CH2 \leq H+C2H$ .00 5.000E+13 .000 C+CH3<=>H+C2H2 5.000E+13 .000 .00 CH+O2<=>O+HCO 6.710E+13 .000 .00 1.080E+14 .000 3110.00  $CH+H2 \leq H+CH2$ CH+H2O<=>H+CH2O 5.710E+12 .000 -755.00  $CH+CH2 \leq H+C2H2$ 4.000E+13 000 00 .00 CH+CH3<=>H+C2H3 3.000E+13 .000 CH+CH4<=>H+C2H4 6.000E+13 .000 .00  $CH+CO(+M) \leq HCCO(+M)$ 5.000E+13 .000 .00 LOW / 2.690E+28 -3.740 1936.00/ TROE/ .5757 237.00 1652.00 5069.00 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ CH+CO2<=>HCO+CO .000 15792.00 1.900E+14 CH+CH2O<=>H+CH2CO 9.460E+13 .000 -515.00 CH+HCCO<=>CO+C2H2 5.000E+13 .000 .00 CH2+O2 =>OH+H+CO5.000E+12 .000 1500.00 CH2+H2<=>H+CH3 5.000E+05 2.000 7230.00 2CH2<=>H2+C2H2 1.600E+15 .000 11944.00 CH2+CH3<=>H+C2H4 4.000E+13 .000 .00 2.460E+06 2.000 8270.00 CH2+CH4<=>2CH3  $CH2+CO(+M) \leq CH2CO(+M)$ 8.100E+11 .500 4510.00 LOW / 2.690E+33 -5.110 7095.00/ TROE/ .5907 275.00 1226.00 5185.00 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ CH2+HCCO<=>C2H3+CO .000 3.000E+13 .00 CH2\*+N2<=>CH2+N2 1.500E+13 .000 600.00 CH2\*+AR<=>CH2+AR 9.000E+12 .000 600.00 CH2\*+O2<=>H+OH+CO 2.800E+13 .000 .00 CH2\*+O2<=>CO+H2O .000 .00 1.200E+13 .000 CH2\*+H2<=>CH3+H .00 7.000E+13  $CH2*+H2O(+M) \leq CH3OH(+M)$ 4.820E+17 -1.160 1145.00 LOW / 1.880E+38 -6.360 5040.00/ TROE/ .6027 208.00 3922.00 10180.0/ H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ CH2\*+H2O<=>CH2+H2O 3.000E+13 .000 .00 CH2\*+CH3<=>H+C2H4 1.200E+13 .000 -570.00 CH2\*+CH4<=>2CH3 1.600E+13 .000 -570.00 .000 CH2\*+CO<=>CH2+CO 9.000E+12 .00 CH2\*+CO2<=>CH2+CO2 7.000E+12 .000 .00 .000 CH2\*+CO2<=>CO+CH2O 1.400E+13 .00 CH2\*+C2H6<=>CH3+C2H5 4.000E+13 .000 -550.00 CH3+O2<=>O+CH3O 3.560E+13 .000 30480.00 CH3+O2<=>OH+CH2O 2.310E+12 .000 20315.00 2.450E+04 2.470 5180.00 CH3+H2O2<=>HO2+CH4  $2CH3(+M) \le C2H6(+M)$ 6.770E+16 -1.180 654.00 LOW / 3.400E+41 -7.030 2762.00/ TROE/ .6190 73.20 1180.00 9999.00/ H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ 2CH3<=>H+C2H5 6.840E+12 .100 10600.00 CH3+HCO<=>CH4+CO 2.648E+13 .000 .00 3.320E+03 2.810 5860.00 CH3+CH2O<=>HCO+CH4 CH3+CH3OH<=>CH2OH+CH4 3.000E+07 1.500 9940.00

1.000E+07 1.500 9940.00 CH3+CH3OH<=>CH3O+CH4 CH3+C2H4<=>C2H3+CH4 2.270E+05 2.000 9200.00 CH3+C2H6<=>C2H5+CH4 6.140E+06 1.740 10450.00 HCO+H2O<=>H+CO+H2O 1.500E+18 -1.000 17000.00  $HCO+M \le H+CO+M$ 1.870E+17 -1.000 17000.00 H2/2.00/ H2O/ .00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ HCO+O2<=>HO2+CO 13.45E+12 .000 400.00 CH2OH+O2<=>HO2+CH2O 1.800E+13 .000 900.00 CH3O+O2<=>HO2+CH2O 4.280E-13 7.600 -3530.00 C2H+O2<=>HCO+CO 1.000E+13 .000 -755.00 C2H+H2<=>H+C2H2 5.680E+10 0.900 1993.00 4.580E+16 -1.390 1015.00 C2H3+O2<=>HCO+CH2O C2H4(+M)<=>H2+C2H2(+M) 8.000E+12 .440 86770.00 LOW / 1.580E+51 -9.300 97800.00/ TROE/ .7345 180.00 1035.00 5417.00 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ C2H5+O2<=>HO2+C2H4 8.400E+11 .000 3875.00 HCCO+O2<=>OH+2CO 3.200E+12 .000 854.00 2HCCO<=>2CO+C2H2 1.000E+13 .000 .00 .000 .00 O+CH3=>H+H2+CO 3.370E+13 O+C2H4<=>H+CH2CHO 3.350E+06 1.830 220.00 ! k opt=0.5\*ko O+C2H5<=>H+CH3CHO 1.096E+14 .000 .00 OH+HO2<=>O2+H2O 0.500E+16 .000 17330.00 DUPLICATE .500 -1755.00 OH+CH3=>H2+CH2O 8.000E+09 1.970E+12 .430 -370.00  $CH+H2(+M) \leq CH3(+M)$ LOW/4.820E+25 -2.80 590.0/ TROE/.578 122.0 2535.0 9365.0 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ CH2+O2=>2H+CO2 5.800E+12 .000 1500.00 CH2+O2<=>O+CH2O 2.400E+12 .000 1500.00 CH2+CH2=>2H+C2H22.000E+14 .000 10989.00 CH2\*+H2O=>H2+CH2O 6.820E+10 .250 -935.00 C2H3+O2<=>O+CH2CHO 1.212E+11 .290 11.00 ! k opt=0.4\*ko C2H3+O2<=>HO2+C2H2 1.337E+06 1.610 -384.00 2.920E+12 O+CH3CHO<=>OH+CH2CHO .000 1808.00 O+CH3CHO=>OH+CH3+CO 2.920E+12 .000 1808.00 O2+CH3CHO=>HO2+CH3+CO 3.010E+13 .000 39150.00 H+CH3CHO<=>CH2CHO+H2 2.050E+09 1.160 2405.00 H+CH3CHO=>CH3+H2+CO 2.050E+09 1.160 2405.00 OH+CH3CHO=>CH3+H2O+CO 2.343E+10 0.730 -1113.00 HO2+CH3CHO=>CH3+H2O2+CO 3.010E+12 .000 11923.00 CH3+CH3CHO=>CH3+CH4+CO 2.720E+06 1.770 5920.00 H+CH2CO(+M)<=>CH2CHO(+M) 4.865E+11 0.422 -1755.00 LOW/ 1.012E+42 -7.63 3854.0/ TROE/ 0.465 201.0 1773.0 5333.0 / H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ O+CH2CHO=>H+CH2+CO2 1.500E+14 .000 .00 1.810E+10 .000 .00 O2+CH2CHO=>OH+CO+CH2O O2+CH2CHO=>OH+2HCO 2.350E+10 .000 .00 H+CH2CHO<=>CH3+HCO 2.200E+13 .000 .00 .000 .00 H+CH2CHO<=>CH2CO+H2 1.100E+13 OH+CH2CHO<=>H2O+CH2CO 1.200E+13 .000 .00

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OH+CH2CHO<=>HCO+CH2OH
                                                           .00
                                       3.010E+13 .000
! File 2a: A set of Oin (commented) & Scott's C3 (C=3) reactions.
١
1=
1
           !
! C3 chemistry
                !
1
           ! ***** C2H3O chemistry and additional reactions for C<3 removed. *****
CH3 + C2H <=> C3H3 + H
                               2.41E+13 0.0
                                               0.0 ! Tsang-Hampson
1
C2H2 + CH \iff C3H2 + H
                               3.00E+13 0.0
                                               0.0 ! Warnatz 83
                               1.20E+13 0.0 6620.0 ! Bohland 86
C2H2 + CH2 \iff C3H3 + H
C2H2 + CH2* \iff C3H3 + H
                                2.00E+13 0.0
                                                0.0 ! Estimated
C2H2 + HCCO \iff C3H3 + CO
                                  1.00E+11 0.0 3000.0 ! Miller-Bowman
1
! ***** Four C1 and C2 reactions removed. *****
! Reactions of C3Hx species
C3H2 + O \iff C2H2 + CO
                                               0.0 ! Warnatz 82
                               6.80E+13 0.0
!C3H2 + OH \iff H + CO + C2H2
                                  6.80E+13 0.0
                                                  0.0 ! Warnatz 82
C3H2 + OH \iff HCO + C2H2
                                 6.80E+13 0.0
                                                 0.0 ! War82 Prod/Miller
!C3H2 + O2 \iff HCCO + H + CO
                                  2.00E+13 0.0
                                                  0.0 ! Miller-Melius
C3H2 + O2 \iff HCCO + H + CO
                                  2.00E+12 0.0 1000.0 ! Miller
C3H2 + H <=> C3H3
                            1.00E+13 0.0
                                            0.0 ! Estimated
۱
! Propargyl Reactions
C3H3 + H \le pC3H4
                             0.855E+13 0.0
                                              0.0 ! Est. ! k opt=0.57*ko
! pC3H4+AR \le C3H3+H+AR
                                 4.7e+18 0.00
                                               80000.
                                                          ! Qin hidaka89
C3H3 + H \le aC3H4
                             0.825E+12 0.0
                                              0.0 ! Est. ! k opt=0.33*ko
! aC3H4+AR \le C3H3+H+AR
                                2.00e+18 0.00 80000.
                                                          ! Oin hidaka89
I
! Products reassigned to avoid C3H3 and C3H2 build-up
1
                               5.00E+13 0.0 1000.0 ! Miller
C3H3 + H \le C3H2 + H2
C3H3 + O \iff CH2O + C2H
                                2.00E+13 0.0
                                                0.0 ! Miller-Bowman
C3H3 + OH <=> C3H2 + H2O
                                                 0.0 ! Miller-Bowman ! k opt=0.71*ko
                                 1.42E+13 0.0
C3H3 + O2 <=> CH2CO + HCO
                                  4.17E+10 0.0 2868.0 ! Gutman ! k_opt=1.39*ko
                                1.1e+12 0.00 9219.
                                                        ! Qin est
! C3H3+O2<=>CH2CO+HCO
C3H3 + HO2 \iff OH + CO + C2H3
                                   8.00E+11 0.0
                                                   0.0 ! Estimated
C3H3 + HO2 <=> aC3H4 + O2
                                                 0.0 ! EST-NEW ! k opt=3*ko
                                9.00E+11 0.0
C3H3 + HO2 \le pC3H4 + O2
                                 1.10E+12
                                           0.0
                                                 0.0 ! EST-NEw ! k opt=0.44*ko
C3H3 + HCO <=> aC3H4 + CO
                                 2.50E+13 0.0
                                                 0.0 ! Estimated
C3H3 + HCO \iff pC3H4 + CO
                                 2.50E+13 0.0
                                                 0.0 ! Estimated
aC3H4 + H \le C3H3 + H2
                               1.30E+06 2.0 5500.0 ! <=> pC3H4 + H
! aC3H4+H<=>C3H3+H2
                              1.00e+12 0.00 1500.
                                                      ! Qin hidaka89
aC3H4 + H <=> CH3CCH2
                               9.46E+42 -9.43 11190.0 ! WD 1 atm
!aC3H4 + H <=> CH3CCH2
                                8.47E+43 -9.59 12462.0 ! WD 2 atm
                                6.98E+44 -9.70 14032.0 ! WD 5 atm
|aC3H4 + H \leq CH3CCH2|
aC3H4 + H \le aC3H5
                             1.52E+59 -13.54 26949.0 ! WD 1 atm
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!aC3H4 + H <=> aC3H5 3.78E+57 -12.98 26785.0 ! WD 2 atm  $|aC3H4 + H| \le aC3H5$ 7.34E+54 -12.09 26187.0 ! WD 5 atm ! aC3H5<=>aC3H4+H 1.40e+13 0.00 59992. ! Oin tsang91 2.00E+07 1.8 1000.0 ! Est. See notes  $aC3H4 + O \le C2H4 + CO$ ! aC3H4+O<=>CO+C2H4 7.8e+12 0.00 1600. ! Oin Westbrook84 ! aC3H4+O<=>HCO+C2H3 1.10e-02 4.613 -4243. ! Qin dagaut92 ! aC3H4+O2<=>C3H3+HO2 4.00e+13 0.00 61500. ! Qin dagaut92 5.30E+06 2.0 2000.0 ! Refit to Liu(note  $aC3H4 + OH \iff C3H3 + H2O$ 3.12e+12 0.00 -397. ! aC3H4+OH<=>CH2CO+CH3 ! Qin dagaut94 2.00e+07 2.00 1000. ! Qin dagaut94 ! aC3H4+OH<=>C3H3+H2O aC3H4 + CH3 <=> C3H3 + CH4 1.30E+12 0.00 7700.0 ! Wu & Kern ! aC3H4+CH3<=>C3H3+CH4 2.00e+12 0.00 7700. ! Qin hidaka89 1.00E+13 0.0  $aC3H4 + C2H \iff C2H2 + C3H3$ 0.0 ! Estimated/ 1.73E+12 0.31 60015.0 ! WD kinf !pC3H4 <=> cC3H4 !pC3H4 <=> cC3H4 2.84E+45 -10.45 69284.0 ! WD 0.4 atm  $pC3H4 \ll cC3H4$ 1.20E+44 -9.92 69250.0 ! WD 1 atm !pC3H4 <=> cC3H4 5.47E+42 -9.43 69089.0 ! WD 2 atm !pC3H4 <=> cC3H4 3.92E+40 -8.69 68706.0 ! WD 5 atm 5.81E+62 -14.63 91211.0 ! WD 0.4 atm !pC3H4 <=> aC3H4 pC3H4 <=> aC3H4 10.3E+60 -13.93 91117.0 ! WD 1 atm ! k opt=2\*ko 7.64E+59 -13.59 91817.0 ! WD 2 atm !pC3H4 <=> aC3H4 3.12E+58 -13.07 92680.0 ! WD 5 atm !pC3H4 <=> aC3H4 2.10e+12 0.00 60000. ! pC3H4<=>aC3H4 ! Qin hidaka89 1.98E+12 0.56 42240.0 ! WD kinf !cC3H4 <=> aC3H4 7.59E+40 -9.07 48831.0 ! WD 0.4 atm  $!cC3H4 \le aC3H4$ cC3H4 <=> aC3H4 4.89E+41 -9.17 49594.0 ! WD 1 atm 8.81E+41 -9.15 50073.0 ! WD 2 atm !cC3H4 <=> aC3H4 4.33E+41 -8.93 50475.0 ! WD 5 atm !cC3H4 <=> aC3H4 1  $pC3H4 + H \le aC3H4 + H$ 6.27E+17 -0.91 10079.0 ! WD 1 atm  $pC3H4 + H \le aC3H4 + H$ 1.50E+18 -1.00 10756.0 ! WD 2 atm 1.93E+18 -1.01 11523.0 ! WD 5 atm  $pC3H4 + H \le aC3H4 + H$  $pC3H4 + H \leq > CH3CCH2$ 1.66E+47 -10.58 13690.0 ! WD 1 atm  $pC3H4 + H \ll CH3CCH2$ 5.04E+47 -10.61 14707.0 ! WD 2 atm 9.62E+47 -10.55 15910.0 ! WD 5 atm  $pC3H4 + H \iff CH3CCH2$  $pC3H4 + H \le aC3H5$ 4.91E+60 -14.37 31644.0 ! WD 1 atm !pC3H4 + H <=> aC3H5 3.04E+60 -14.19 32642.0 ! WD 2 atm !pC3H4 + H <=> aC3H5 9.02E+59 -13.89 33953.0 ! WD 5 atm 1.15E+08 1.9 7530.0 ! <=> C2H6 + H  $!pC3H4 + H \le C3H3 + H2$ 1.30E+06 2.0 5500.0 ! Estimated (from Wu and Kern)  $pC3H4 + H \le C3H3 + H2$ 1500. ! pC3H4+H<=>C3H3+H2 1.0e+12 0.00 ! Qin hidaka89 ! pC3H4+H<=>C2H2+CH3 1.30e+05 2.5 1000. ! Qin hidaka89  $pC3H4 + C3H3 \iff aC3H4 + C3H3$ 6.140E+06 1.740 10450. ! Estimate(CH3+C2H6)  $pC3H4 + H \le CH3 + C2H2$ 1.30E+05 2.5 1000.0 ! Hidaka 2.04E+13 0.0 2250.0 ! Fontijn/split ! k opt=2.79\*ko  $pC3H4 + O \iff HCCO + CH3$ ! pC3H4+O<=>HCCO+CH3 6.30e+12 0.00 2010. ! Qin dagaut94 0.58E+13 0.0 2250.0 ! Fontijn/split ! k opt=0.58\*ko  $pC3H4 + O \iff C2H4 + CO$  $pC3H4 + O \iff C2H3 + HCO$ 0.73E+13 0.0 2250.0 ! Fontijn/split ! pC3H4+O<=>C2H3+HCO 3.20e+12 0.00 2010. ! Qin dagaut94  $pC3H4 + O \iff C3H3 + OH$ 3.45e+04 2.16 4830.0 ! Fontijn ! pC3H4+O<=>CH2CO+CH2 6.40e+12 0.00 2010. ! Qin dagaut94 ! pC3H4+O2<=>C3H3+HO2 5.00e+12 0.00 51000. ! Qin dagaut94

$!pC3H4 + OH <=> C3H3 + H2O \qquad 3.54E+06  2.12  870.0  ! <=> C2H6 + OH \text{ (too high)}$
pC3H4 + OH <=> C3H3 + H2O 1.00E+06 2.0 100.0 ! This work
! pC3H4+OH<=>C3H3+H2O 2.00e+07 2.00 1000. ! Qin_dagaut94
! pC3H4+OH<=>CH2CO+CH3 5.00e-04 4.50 -1000. ! Qin_dagaut94
pC3H4 + C2H <=> C2H2 + C3H3 1.00E+13 0.0 0.0 ! Estimated
pC3H4 + CH3 <=> C3H3 + CH4 1.80E+12 0.0 7700.0 ! Wu & Kern
pC3H4+CH3<=>C3H3+CH4 2.00e+12 0.00 7700. ! Qin hidaka89
!
!
! Reactions of propane
!
$C3H8+H \le H2+nC3H7$ 1.30E+06 2.54 6756.0 ! TS3
C3H8+H $\leq H2+iC3H7$ 2.60E+06 2.40 4471.0 ! TS3 ! k_opt=2*ko
! C3H8+H<=>iC3H7+H2 1.26e+08 1.735 4864. ! Qin_yang98
! C3H8+H<=>nC3H7+H2 1.95e+08 1.827 7463. ! Qin_yang98
$C3H8+O \le nC3H7+OH$ 1.90E+05 2.68 3716.0 ! TS3
C3H8+O <=> iC3H7+OH 4.76E+04 2.71 2106.0 ! TS3
! C3H8+O<=>iC3H7+OH 4.77e+04 2.71 2106. ! Qin_tsang88
! C3H8+O<=>nC3H7+OH 1.93e+05 2.68 3716. ! Qin tsang88
C3H8+OH <=> nC3H7+H2O 1.40E+03 2.66 527.0 ! TS3
C3H8+OH <=> iC3H7+H2O 2.70E+04 2.39 393.0 ! TS3
! C3H8+OH<=>iC3H7+H2O 1.84e+05 2.38 -573. ! Qin dagaut92
! C3H8+OH<=>nC3H7+H2O 4.16e+07 1.74 540. ! Oin dagaut92
$C3H8+O2 \le nC3H7+HO2$ 4.00E+13 0.00 50930.0 ! TS3
$C3H8+O2 \le iC3H7+HO2$ 4.00E+13 0.00 47590.0 1 TS3
C3H8+O2  =>  C3H7+HO2  = 3.97e+13 = 0.00 = 47688  Oin tsang88
$1C_{3H8+O2} = nC_{3H7+HO2} = 3.97e+13 = 0.00 = 50867 = 1.0in tsang88$
C3H8+HO2 <=> nC3H7+H2O2  476F+04  255  16490  0.1 TS3
C3H8+HO2 <=>iC3H7+H2O2 964F+O3 260 13910.0 1TS3
$1 C_{3H8+HO2} <=>iC_{3H7+H2O2} = 9.642+03 - 2.60 - 13910.0 + 155$
$1 C_{3H8+HO2} <=>nC_{3H7+H2O2} = 1.050(+05-2.00+15)(5). 1 C_{1} C_{1}$
$C_{2H8+CH3} <=> CH4+nC_{2H7} = 0.03E_{01} = 3.65 = 7153.0 \pm TS3$
C3H8+CH3 <=> CH4+iC3H7 = 1.51E+00 = 3.46 = 5.480.0 + 1.53
$1 CH_{2} C_{2}H_{2} = -iC_{2}H_{7} C_{1}H_{1} = 1.512 \pm 00.3.46 = 5480.0 \pm 1.55$
1 CH3 + C3H8 < ->nC3H7 + CH4 = 1.510 + 00 3.40 5460. $1 CH3 + C3H8 < ->nC3H7 + CH4 = 0.03 + 01 - 2.65 - 7153 = 1.0in tranges$
$1 C_{112} = C_$
$2C_{13}+C_{310} < -2C_{14}+C_{317} = (0.25+0.2, 2.20, 10501) = 10in trans00$
2CH5+C5H8 <= 2C2H4+nC5H7 = 0.050+02 5.50 10501. 2011 [Sang88]
2C2H5+C3H8 <= 2C2H0+1C3H7 1.200+00 3.40 /407. $2C112 C2H5+C2H0 <= 2C2H0+1C3H7$ 1.200+00 3.40 /407. $2C112 C2H5+C2H0 <= 2C2H0+1C3H7$
$2C_{H5}+C_{H6}=2C_{H6}+nC_{H7}$ 9.04e-01 3.65 9140. $2C_{H6}=101$ tsang88
2.5H8+aC3H5 <= >HC3H7+C3H6 /.8/6+01 3.50 18109. 201 [sang9]
$!C_{3H8+aC_{3H5}<=>nC_{3H7+C_{3H6}}$ 2.35e+02 3.30 19842. !Qin_tsang91
$103H/+C3H8 \le nC3H/+C3H8 = 8.44e-03 4.20 8684. 101 tsang88$
! CH3O+C3H8<=>CH3OH+iC3H/ 1.45e+11 0.00 45/0. ! Qin_tsang88
$! CH3O+C3H8 \le CH3OH+nC3H7 4.34e+11 0.00 6458. ! Qin_tsang88$
! Reactions of n-propyl
! nC2H7+H(+M) < -> C2H8(+M) = 2.60E+12 = 0.00 = 0.0 + TS2.600  cm = 1
$ICSIT/TI(TW) \sim CSII8(TW) = 5.00E TIS 0.00 = 0.0 + 155 000 CIII-1 = 1 OW / 2.01E + 49 0.22 5922.6 /$
$\frac{1}{1000} + \frac{1}{1000} + \frac{1}{1000} + \frac{1}{1000} + \frac{1}{10000} + \frac{1}{10000} + \frac{1}{100000} + \frac{1}{10000000} + \frac{1}{10000000000000000000000000000000000$
IROE / 0.498 IS14.0 IS14.0 S0000.0 / H2/2/ H2O/6/ CH4/2/ CO/1 5/ CO2/2/ C2H6/2/ AD/0 7/
$\frac{112}{2} \frac{112}{112} \frac{112}{10} \frac{10}{100} \frac{114}{2000} \frac{100}{1000} \frac{1000}{10000000000000000000000000000000$
$U_{2114/3.07}$ $P_{0.014/4.07}$ $U_{0.010/4.07}$ $U_{0.010/4.07}$ $U_{0.010/4.07}$ $U_{0.010/4.07}$ $U_{0.010/4.07}$ $U_{0.010/4.07}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\frac{10000}{1000000000000000000000000000000$
1 ST 1 ST 2 ST 2 ST 2 ST 2 ST 2 ST 2 ST
1

```
nC3H7+H <=> C3H6+H2
                            1.80E+12 0.00
                                             0.0 ! TS3
nC3H7+O <=> C2H5+CH2O
                              9.60E+13 0.00
                                              0.0 ! TS3 ka+kb
nC3H7+OH <=> C3H6+H2O
                              2.40E+13 0.00
                                              0.0 ! TS3
                              9.00E+10 0.00
                                              0.0 ! TS3
nC3H7+O2 <=> C3H6+HO2
! nC3H7+O2<=>C3H6+HO2
                              1.00e+12 0.00 5019.
                                                      ! Oin tsang88
nC3H7+HO2 \iff C2H5+OH+CH2O
                                  2.40E+13 0.00
                                                   0.0 ! TS3
nC3H7+HCO \iff C3H8+CO
                              6.00E+13 0.00
                                               0.0 ! TS3
nC3H7+CH3 <=> CH4+C3H6
                               1.10E+13 0.00
                                               0.0 ! TS3
! kinf : TS3 recommendation
! ko: scaled such that Pr(nC3H7+CH3) \leq Pr(C2H5+CH3) = 500cm-1
! Fc: assumed equal to Fc(C2H5+CH3)
۱
! Reactions of i-propyl
۱
iC3H7+H(+M) \le C3H8(+M)
                              2.40E+13 0.00
                                               0.0 ! TS3 600 cm-1
           LOW / 1.70E+58 -12.08 11263.7
                                           /
           TROE / 0.649 1213.1 1213.1 13369.7 /
  H2/2/H2O/6/CH4/2/CO/1.5/CO2/2/C2H6/3/AR/0.7/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
                             5.90E+23 -2.81 10009.0 ! TS3 0.1 atm
!iC3H7+H <=> CH3+C2H5
iC3H7+H <=> CH3+C2H5
                             1.40E+28 -3.94 15916.0 ! TS3 1 atm
!iC3H7+H <=> CH3+C2H5
                             4.00E+24 -2.83 17542.0 ! TS3 10 atm
1
iC3H7+H <=> C3H6+H2
                            3.20E+12 0.00
                                            0.0 ! TS3
iC3H7+O <=> CH3CHO+CH3
                               9.60E+13 0.00
                                              0.0 ! TS3 ka+kb
                              2.40E+13 0.00
                                              0.0 ! TS3
iC3H7+OH \iff C3H6+H2O
iC3H7+O2 <=> C3H6+HO2
                             1.30E+11 0.00
                                              0.0 ! TS3
                              1.26e+11 0.00
! iC3H7+O2<=>C3H6+HO2
                                                    ! Qin tsang88
                                              0.
iC3H7+HO2 <=> CH3CHO+CH3+OH 2.40E+13
                                             0.00
                                                    0.0 ! TS3
                              1.20E+14 0.00
                                              0.0 ! TS3
iC3H7+HCO \iff C3H8+CO
iC3H7+CH3 <=> CH4 + C3H6
                              2.20E+14 -0.68
                                              0.0 ! TS3
١
! Reactions of propene
1
C3H6+H(+M) \le nC3H7(+M)
                               1.33E+13 0.00 3260.7 ! TS5 600 cm-1
           LOW / 6.26E+38 -6.66 7000.0
                                          /
            TROE / 1.000 1000.0 1310.0 48097.0 /
  H2/2/H2O/6/CH4/2/CO/1.5/CO2/2/C2H6/3/AR/0.7/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
! nC3H7<=>H+C3H6
                           1.26e+14 0.00 37000.
                                                   ! Qin westbrook84
! nC3H7<=>CH3+C2H4
                            1.20e+13 0.00 30300.
                                                     ! Oin tsang88
C3H6+H(+M) \le iC3H7(+M)
                              1.33E+13 0.00 1559.8 ! TS5 600cm-1
           LOW / 8.70E+42 -7.50 4721.8
            TROE / 1.000 1000.0 645.4 6844.3 /
  H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
! iC3H7<=>H+C3H6
                          1.60e+13 0.00 35766.
                                                  ! Oin tsang88
! iC3H7<=>CH3+C2H4
                            2.00e+10 0.00 29500.
                                                    ! Qin westbrook84
!C3H6+H <=> C2H4+CH3
                             17.6E+16 -1.05 6461.0 ! TS5 0.1 atm*2
                             25.76E+21 -2.39 11180.0 ! TS5 1 atm*2 ! k opt=1.61*ko
C3H6+H <=> C2H4+CH3
!C3H6+H <=> C2H4+CH3
                             6.60E+24 -3.04 15610.0 ! TS5 10 atm*2
! C3H6+H<=>CH3+C2H4
                              7.23e+12 0.00 1301.
                                                    ! Qin tsang91
١
C3H6+H <=> aC3H5+H2
                            0.85E+05 2.50 2490.0 ! TS5 k(a) ! k opt=0.5*ko
```

1.70e+05 2.50 2492. ! C3H6+H<=>aC3H5+H2 ! Qin tsang92  $C3H6+H \iff CH3CCH2+H2$ 4.00E+05 2.50 9790.0 ! TS5 k(b) C3H6+O <=> CH2CO+CH3+H 1.20E+08 1.65 327.0 ! TS5 k(a+b) tot 3.50E+07 1.65 -972.0 ! TS5 k(c) C3H6+O <=> C2H5+HCO ! C3H6+O<=>C2H5+HCO 1.20e+11 0.70 8959. ! Oin tsang91 C3H6+O <=> aC3H5+OH 1.80E+11 0.70 5880.0 ! TS5 k(d) C3H6+O <=> CH3CCH2+OH 6.00E+10 0.70 7630.0 ! TS5 K(f) 5.89e+13 0.00 5000. ! Qin westbrook84 ! C3H6+O<=>C2H4+CH2O 1.17e+13 0.00 600. ! Qin westbrook84 ! C3H6+O<=>CH3+CH3+CO 3.97E+06 2.00 -298.0 ! TS5 ! k opt=1.28\*ko C3H6+OH <=> aC3H5+H2O C3H6+OH <=> CH3CCH2+H2O 1.10E+06 2.00 1450.0 ! TS5 ! C3H6+OH<=>C2H5+CH2O 7.90e+12 0.00 0. ! Qin cathonnet81 3.47e+11 0.00 ! Qin westbrook84 ! C3H6+OH<=>CH3+CH3CHO 0.  $! C3H6+OH \le aC3H5+H2O$ 3.12e+06 2.00 -298. ! Oin tsang91 2.14e+06 2.00 2778. ! Qin tsang91 ! C3H6+OH<=>CH3CHCH+H2O ! C3H6+OH<=>CH3CCH2+H2O 1.11e+06 2.00 1451. ! Qin tsang91 ! CH3CHCH+H<=>aC3H4+H2 3.33e+12 0.00 0. ! Qin dagaut88 ! CH3CHCH+O<=>CH2CO+CH3 1.807e+14 0.00 0. ! Qin dagaut88 ! CH3CHCH+CH3<=>aC3H4+CH4 1.000e+11 0.00 0. ! Qin dagaut88 ! CH3CHCH+C2H3<=>aC3H4+C2H4 1.000e+11 0.00 0. ! Qin dagaut88 0. ! Qin dagaut88 ! CH3CHCH+C2H5<=>aC3H4+C2H6 1.000e+11 0.00 ! CH3CCH2+H<=>aC3H4+H2 3.33e+12 0.00 0. ! Qin dagaut88 C3H6+HO2 <=> aC3H5+H2O2 9.60E+03 2.60 13910.0 ! TS5 2.20E+00 3.50 5675.0 ! TS5 k(c) C3H6+CH3 <=> aC3H5+CH4 ! C3H6+CH3<=>aC3H5+CH4 2.21e+00 3.50 5675. ! Oin tsang91 C3H6+CH3 <=> CH3CCH2+CH4 8.40E-01 3.50 11660.0 ! TS5 k(e) ! C3H6+C2H5<=>aC3H5+C2H6 2.23e+00 3.50 6637. ! Qin tsang91 1 ! Reactions of allyl  $aC3H5+H(+M) \le C3H6(+M)$ 3.70E+14 0.00 0.0 ! TS5 600cm-1 ! k opt=1.85\*ko LOW / 1.33E+60 -12.00 5967.8 TROE / 0.020 1096.6 1096.6 6859.5 / H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ ! C3H6<=>aC3H5+H 2.50e+15 0.00 86679. ! Qin tsang91 ! aC3H5+H <=> aC3H4+H2 1.80E+13 0.00 0.0 ! TS5 k(c)! aC3H5+H<=>aC3H4+H2 1.81e+13 0.00 0. ! Oin tsang91 aC3H5+O <=> C2H3CHO+H 6.00E+13 0.00 0.0 ! TS5 !aC3H5+OH <=> C2H3CHO+H+H 5.30E+37 -6.71 29306.0 ! TS5, 0.1 atm aC3H5+OH <=> C2H3CHO+H+H 4.20E+32 -5.16 30126.0 ! TS5, 1 atm !aC3H5+OH <=> C2H3CHO+H+H 1.60E+20 -1.56 26330.0 ! TS5, 10 atm 1 C2H3+HCO <=> C2H3CHO 1.80E+13 0.00 0.0 ! TS5 C2H3CHO+H <=> C2H4+HCO 1.08E+12 0.454 1820.00 ! <=>C2H4+H (kinf) C2H3CHO+O <=> C2H3+OH+CO 3.00E+13 0.00 3540.00 ! <=>CH2O+O C2H3CHO+O <=> CH2O+CH2CO 1.90E+07 1.80 220.00 ! <=>C2H4+O C2H3CHO+OH <=> C2H3+H2O+CO 3.43E+09 1.18 -447.00 ! <=>CH2O+OH I  $aC3H5+OH \le aC3H4+H2O$ 6.00E+12 0.00 0.0 ! TS5 k(a)4.99E+15 -1.40 22428.0 ! Bozzelli, 1 atm aC3H5+O2 <=> aC3H4+HO2 !aC3H5+O2 <=> aC3H4+HO2 2.18E+21 -2.85 30755.0 ! Bozzelli, 10 atm ! aC3H5+O2<=>aC3H4+HO2 1.21e+12 0.00 13551. ! Qin tsang91 1.19E+15 -1.01 20128.0 ! Bozzelli, 1 atm aC3H5+O2 <=> CH3+CO+CH2O !aC3H5+O2 <=> CH3+CO+CH2O 7.14E+15 -1.21 21046.0 ! Bozzelli, 10 atm

```
aC3H5+O2 <=> C2H3CHO+OH
                               1.82E+13 -0.41 22859.0 ! Bozzelli, 1 atm
!aC3H5+O2 <=> C2H3CHO+OH
                               2.47E+13 -0.45 23017.0 ! Bozzelli, 10 atm
I
aC3H5+HO2 \iff C3H6+O2
                             2.66E+12 0.00
                                             0.0 ! CEC
aC3H5+HO2 \iff OH+C2H3+CH2O
                                 6.60E+12 0.00
                                                  0.0 ! CEC
!aC3H5+HO2 <=> OH+C2H3+CH2O
                                 3.00E+12 0.00
                                                  0.0 ! CEC/2.21
1
aC3H5+HCO <=> C3H6+CO
                              6.00E+13 0.00
                                              0.0 ! TS5
١
                              3.00E+12 -0.32 -131.0 ! TS5 k(a)
aC3H5+CH3 <=> aC3H4+CH4
                                3.01e+12 -0.32 -131.
! aC3H5+CH3<=>aC3H4+CH4
                                                     ! Oin tsang91
aC3H5+aC3H5 <=> C3H6 + aC3H4 1.00E+13 0.00
                                              0.0 ! Estimated
                           7.06E+56 -14.08 75868.0 ! WD 1 atm
aC3H5 <=> CH3CCH2
                           4.80E+55 -13.59 75949.0 ! WD 2 atm
!aC3H5 <=> CH3CCH2
                           4.86E+53 -12.81 75883.0 ! WD 5 atm
!aC3H5 <=> CH3CCH2
! aC3H5+C2H3<=>aC3H4+C2H4
                                  2.41+12\ 0.00\ 0.
                                                     ! Qin tsang91
! aC3H5+C2H3<=>C3H6+C2H2
                                 4.82+12 0.00 0.
                                                     ! Oin tsang91
! aC3H5+C2H5<=>aC3H4+C2H6
                                  9.64e+11 0.00 -131. ! Qin tsang91
! aC3H5+C2H5<=>C3H6+C2H4
                                 2.59e+12 0.00 -131.
                                                      ! Qin tsang91
! Reactions of propen-2-yl
۱
CH3CCH2+H <=> pC3H4+H2
                               3.34E+12 0.00
                                                0.0 ! PW
CH3CCH2+O <=> CH3+CH2CO
                                                 0.0 ! Estimated
                                 6.00E+13 0.00
CH3CCH2+OH <=> CH3+CH2CO+H
                                    5.00E+12 0.00
                                                    0.0 ! Estimated
!CH3CCH2+O2 <=> CH3CHO+HCO
                                   1.00E+11 0.00
                                                   0.0 ! PW/changed
CH3CCH2+O2 <=> CH3+CO+CH2O
                                   1.00E+11 0.00
                                                   0.0 ! PW/changed
CH3CCH2+HO2 <=> CH3+CH2CO+OH
                                     2.00E+13 0.00
                                                     0.0 ! Estimated
CH3CCH2+HCO <=> C3H6+CO
                                 9.00E+13 0.00
                                                 0.0 ! Estimated
CH3CCH2+CH3 <=> pC3H4+CH4
                                  1.00E+11 0.00
                                                  0.0 ! PW
١
 ***** Five reactions of CH3CHO removed. *****
١
۱
 ***** Eight reactions of CH3CO removed. *****
! Recombination reactions of C1 and C2 species
! ***** Reaction CH3+HCO <=> CH3CHO removed. *****
١
CH3+C2H2 <=> pC3H4+H
                          1.28E+09 1.10 13644.0 ! WD 1 atm ! k opt=0.5*ko
!CH3+C2H2 <=> pC3H4+H
                          2.07E+10 0.85 14415.0 ! WD 2 atm
!CH3+C2H2 <=> pC3H4+H
                          2.51E+11 0.56 15453.0 ! WD 5 atm
CH3+C2H2 <=> aC3H4+H
                          5.14E+09 0.86 22153.0 ! WD 1 atm
!CH3+C2H2 <=> aC3H4+H
                          1.33E+10 0.75 22811.0 ! WD 2 atm
!CH3+C2H2 <=> aC3H4+H
                          9.20E+10 0.54 23950.0 ! WD 5 atm
CH3+C2H2 <=> CH3CCH2
                           4.99E+22 -4.39 18850.0 ! WD 1 atm
!CH3+C2H2 <=> CH3CCH2
                           6.00E+23 -4.60 19571.0 ! WD 2 atm
                           7.31E+25 -5.06 21150.0 ! WD 5 atm
!CH3+C2H2 \iff CH3CCH2
                        2.68E+53 -12.82 35730.0 ! WD 1 atm
CH3+C2H2 \iff aC3H5
                        3.64E+52 -12.46 36127.0 ! WD 2 atm
!CH3+C2H2 <=> aC3H5
!CH3+C2H2 <=> aC3H5
                         1.04E+51 -11.89 36476.0 ! WD 5 atm
CH3+C2H3(+M) \le C3H6(+M)
                               2.50E+13 0.00
                                               0.0 ! TS1 600cm-1
           LOW / 4.27E+58 -11.94 9769.8
```

```
TROE / 0.175 1340.6 60000.0 10139.8 /
 H2/2/H2O/6/CH4/2/CO/1.5/CO2/2/C2H6/3/AR/0.7/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
! C3H6<=>C2H3+CH3
                          8.39e+14 0.00 87990.
                                                ! Qin hidaka92
1
!CH3+C2H3 <=> aC3H5+H
                            1.00E+36 -6.28 22442.0 ! TS1 0.1 atm
                            1.50E+24 -2.83 18618.0 ! TS1 1 atm
CH3+C2H3 <=> aC3H5+H
!CH3+C2H3 <=> aC3H5+H
                            3.00E+08 1.65 12027.0 ! TS1 10 atm
1
                          3.30E+11 0.00 7700.0 ! KP
CH3+C2H4 <=> nC3H7
CH3+C2H5(+M) \le C3H8(+M)
                              9.60E+14 -0.50
                                             0.0 ! TS3 TS1 500cm-1 ! k_opt=1.96*ko
           LOW / 6.80E+61 -13.42 6000.0

           TROE / 1.000 1000.0 1433.9 5328.8 /
  H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
! C3H8<=>CH3+C2H5
                           2.58d+232 -60.2 254600. ! Qin 2.6 to 4.2 atm
!C2H3+C2H5 <=> aC3H5+CH3
                              8.00E+25 -3.46 11775.0 ! TS1 0.1 atm
C2H3+C2H5 <=> aC3H5+CH3
                             3.90E+32 -5.22 19747.0 ! TS1 1 atm
!C2H3+C2H5 <=> aC3H5+CH3
                              3.90E+29 -4.24 22311.0 ! TS1 10 atm
! File 3a: A set of Scott's C>3 (C \leq 4, 5, 6) reactions.
1
!
! C4-up chemistry !
                                     !
1
C2H2 + C2H \iff C4H2 + H
                             9.60E+13 0.0 0.0 ! See notes
                            4.50E+37 -7.68 7100.0 ! RRKM, 760 t
C2H2 + C2H \iff n-C4H3
                            2.60E+44 -9.47 14650.0 ! RRKM, 760 t
C2H2 + C2H \le i-C4H3
C2H2 + C2H3 \iff C4H4 + H
                              2.00E+18 -1.68 10600. ! 760 t
                             9.3E+38 -8.76 12000. ! 760 t
C2H2 + C2H3 \iff n-C4H5
C2H2 + C2H3 \iff i-C4H5
                             1.6E+46 -10.98 18600. ! 760 t
C2H4 + C2H \iff C4H4 + H
                             1.20E+13 0.0
                                             0.0 ! Tsang
                              2.8E+21 -2.44 14720.0 ! 760 t
C2H4 + C2H3 \iff C4H6 + H
                            1.5E+42 -8.84 12483. ! RRKM 760 t
C2H3 + C2H3 \iff C4H6
                             1.2E+22 -2.44 13654. ! RRKM 760 t
C2H3 + C2H3 \iff i-C4H5 + H
C2H3 + C2H3 \iff n-C4H5 + H
                              2.4E+20 -2.04 15361. ! RRKM 760 t
! Reactions of C3Hx species
C3H2 + CH \le C4H2 + H
                             5.00E+13 0.0
                                            0.0 ! Estimated
                                            0.0 ! Estimated
C3H2 + CH2 \iff n-C4H3 + H
                              5.00E+13 0.0
C3H2 + CH3 \iff C4H4 + H
                             5.00E+12 0.0
                                             0.0 ! Estimated
C3H2 + HCCO \iff n-C4H3 + CO
                                1.00E+13 0.0
                                               0.0 ! Estimated
1
! Products reassigned to avoid C3H3 and C3H2 build-up
0.0 ! Estimated
C3H3 + HCCO \iff C4H4 + CO
                               2.50E+13 0.0
C3H3 + CH \le i-C4H3 + H
                                            0.0 ! Estimated
                             5.00E+13 0.0
C3H3 + CH2 \iff C4H4 + H
                             5.00E+13 0.0
                                           0.0 ! Estimated
                             2.00E+13 0.0 2000.0 ! Estimated
i-C4H5 + H \le C3H3 + CH3
C3H3 + CH3 (+M) \le C4H612 (+M) \quad 1.50E+12 \quad 0.0
                                               0.0 ! kinf assumed falloff<=>C2H3+CH3
TS1 600 cm-1
            LOW /2.60E+57 -11.94 9770.0/
```

```
TROE /0.175 1340.6 60000.0 9769.8/
 H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
!
A1 - pC3H4 \le A1 + C3H3
                               2.000E+12 0.0 15000.0
A1 - + aC3H4 \le A1 + C3H3
                               2.000E+12 0.0 15000.0
1
! Reactions of C4H2
1
                             1.10E+42 -8.72 15300.0 ! RRKM, 760 t
C4H2 + H \le n-C4H3
C4H2 + H \le i-C4H3
                            1.10E+30 -4.92 10800.0 ! RRKM, 760 t
C4H2 + O \iff C3H2 + CO
                               2.70E+13 0.0 1720.0 ! Wellman
C4H2 + OH \iff H2C4O + H
                                6.60E+12 0.0 -410.0 ! Perry?
                                 5.00E+13 0.0 3000.0 ! Miller-Melius
H2C4O + H \leq 2C2H2 + HCCO
H2C4O + OH \iff CH2CO + HCCO
                                    1.00E+07 2.0 2000.0 ! Miller-Melius
! Reactions of C4H3 and C4H4
1
n-C4H3 <=> i-C4H3
                           4.10E+43 -9.49 53000.0 ! RRKM, 760 t
n-C4H3 + H \le i-C4H3 + H
                               2.50E+20 -1.67 10800.0 ! RRKM, 760 t
n-C4H3 + H \le C2H2 + C2H2
                                6.30E+25 -3.34 10014.0 ! RRKM, 760 t
i-C4H3 + H \le C2H2 + C2H2
                                2.80E+23 -2.55 10780.0 ! RRKM, 760 t
n-C4H3 + H \le C4H4
                             2.00E+47 -10.26 13070.0 ! RRKM, 760 t
                            3.40E+43 -9.01 12120.0 ! RRKM, 760 t
i-C4H3 + H <=> C4H4
n-C4H3 + H \le C4H2 + H2
                               3.00E+13 0.00 0.0 ! 0.5*C2H3+H
i-C4H3 + H \le C4H2 + H2
                               6.00E+13 0.00
                                              0.0 ! C2H3+H
n-C4H3 + OH \iff C4H2 + H2O
                                 2.00E+12 0.00 0.0
i-C4H3 + OH \le C4H2 + H2O
                                4.00E+12 0.00 0.0
i-C4H3 + O2 \iff HCCO + CH2CO
                                  7.86E+16 -1.80 0.0 ! Gutman
1
                             1.3E+51 -11.92 16500. ! 760 t
C4H4 + H \le n-C4H5
C4H4 + H <=> i-C4H5
                             4.9E+51 -11.92 17700. ! 760 t
C4H4 + H \le n-C4H3 + H2
                               6.65E+05 2.53 12240.0 ! <=>(C2H4+H)/2
C4H4 + H \le i-C4H3 + H2
                              3.33E+05 2.53 9240.0 ! -3kcal/mol. /4
C4H4 + OH \iff n-C4H3 + H2O
                                 3.10E+07 2.0 3430.0 ! <=> C4H6 + OH
                                1.55E+07 2.0 430.0 ! -3kcal/mol, /2
C4H4 + OH \le i-C4H3 + H2O
١
! Reactions of C4H5 and 1,3-C4H6
1
n-C4H5 <=> i-C4H5
                            1.5E+67 -16.89 59100. ! 760 t
n-C4H5 + H \le i-C4H5 + H
                              3.1E+26 -3.35 17423. ! RRKM 760 t
C4H6 <=> i-C4H5 + H
                            5.7E+36 -6.27 112353. ! RRKM 760 t
C4H6 <=> n-C4H5 + H
                            5.3E+44 -8.62 123608. ! RRKM 760 t
                               1.5E+13 0.00
n-C4H5 + H \le C4H4 + H2
                                              0
                               3.0E+13 0.00
i-C4H5 + H \le C4H4 + H2
                                               0.
n-C4H5 + OH <=> C4H4 + H2O
                                 2.0E+12 0.00 0.
i-C4H5 + OH \iff C4H4 + H2O
                                 4.0E+12 0.00
                                                 0.
n-C4H5 + O2 \le C2H4 + CO + HCO = 4.16E+10 = 0.00 = 2500. ! Gutman
i-C4H5 + O2 \iff CH2CO + CH2CHO
                                     7.86E+16 -1.80 0.0 ! <=>i-C4H3+O2
n-C4H5 + HCO \le C4H6 + CO
                                  9.00E+13 0.0
                                                  0. ! Estimated
i-C4H5 + HCO \le C4H6 + CO
                                 9.00E+13 0.0
                                                 0. ! Estimated
1
                               1.33E+06 2.53 12240.0 ! <=> C2H4 + H
C4H6 + H \le n-C4H5 + H2
                               6.65E+05 2.53 9240.0 ! -3kcal/mol,/2
C4H6 + H \le i - C4H5 + H2
                               7.00E+12 0.0 2000.0 ! Est.
C4H6 + H \le pC3H4 + CH3
C4H6+O <=> HCO+aC3H5
                                6.00E+08 1.45 -860.0 ! Fontijn
```

```
6.20E+06 2.0 3430.0 ! refit to Liu
C4H6 + OH \le n-C4H5 + H2O
C4H6 + OH \iff i-C4H5 + H2O
                                 3.10E+06 2.0 430.0 ! -3kcal/mol
1
! Reactions of 1,2-C4H6
C4H612 + H \le C4H6 + H
                               2.00E+13 0.0 4000.0 ! Estimated
                                1.70E+05 2.5 2490.0 ! <=> C3H6+H TS5
C4H612 + H \le i-C4H5 + H2
C4H612 + H <=> aC3H4 + CH3
                                 2.00E+13 0.0 2000.0 ! Estimated
C4H612 + H <=> pC3H4 + CH3
                                 2.00E+13 0.0 2000.0 ! Estimated
C4H612 + O <=> CH2CO + C2H4
                                  1.20E+08 1.65 327.0 ! C3H6+O TS5
C4H612 + O \le i-C4H5 + OH
                                1.80E+11 0.70 5880.0 ! C3H6+O TS5
C4H612 + OH <=> i-C4H5 + H2O
                                 3.10E+06 2.00 -298.0 ! C3H6+OH
                            1.00E+13 0.0 65000.0 ! Estimated
C4H612 <=> C4H6
۱
! Reactions up to benzene formation and oxidation
!
١
C4H2 + C2H \iff C6H2 + H
                               9.60E+13 0.0 0.0 ! <=> C2H2 + C2H
C4H2 + C2H \iff C6H3
                              4.50E+37 -7.68 7100.0 ! RRKM, 760 t
C3H3 + C3H3 <=> A1- + H
                               10.20E+12 0.0 0.0 ! k opt=2.04*ko
                             5.780E+12 0.0 0.0 ! k opt=2.89*ko
C3H3 + C3H3 \iff A1
n-C4H3 + C2H2 <=> 1-C6H4 + H
                                 2.5E+14 -0.56 10600. ! 760 t
n-C4H3 + C2H2 <=> A1-
                              9.6E+70 -17.77 31300. ! 760 t
                                 6.9E+46 -10.01 30100. ! 760 t
n-C4H3 + C2H2 \le c-C6H4 + H
C4H4 + C2H \le l-C6H4 + H
                                1.20E+13 0.0
                                              0.0 ! \le C2H+C2H4
n-C4H5 + C2H2 \iff A1 + H
                                1.6E+16 -1.33 5400. ! 760 t
1
! Reactions of C6H2
1
C6H2 + H <=> C6H3
                            1.10E+30 -4.92 10800.0 ! RRKM, 760 t
١
! Reactions of C6H3 and C6H4
1
C6H3 + H \le C4H2 + C2H2
                                2.80E+23 -2.55 10780.0 ! RRKM, 760 t
C6H3 + H \le 1-C6H4
                            3.40E+43 -9.01 12120.0 ! RRKM, 760 t
C6H3 + H \le C6H2 + H2
                              3.00E+13 0.00 0.0 ! C2H3+H
C6H3 + OH \le C6H2 + H2O
                                4.00E+12 0.00 0.0
                                   5.00E+11 0.00 0.0 ! Estimated
C6H3+O2 \iff CO+C3H2+HCCO
I-C6H4 + H <=> A1-
                            1.7E+78 -19.72 31400. ! 760 t
1-C6H4 + H \le c-C6H4 + H
                               1.4E+54 -11.70 34500. ! 760 t
                               1.33E+06 2.53 9240.0 ! <=> C4H4+H
1-C6H4 + H \le C6H3 + H2
1-C6H4 + OH \iff C6H3 + H2O
                                 3.10E+06 2.0 430.0 ! see notes
c-C6H4 + H <=> A1-
                            2.4E+60 -13.66 29500. ! 760 t
١
! Reactions of benzene and phenyl
۱
A1 + H \le A1 - H2
                            2.50E+14 0.0 16000. ! Kiefer
A1 + OH \le A1 - H2O
                              1.60E+08 1.42 1450.0 ! CEC
A1 - + H (+M) \le A1 (+M)
                               1.0E+14 0.00
                                               0.
  LOW/6.6E+75 -16.30 7000./
  TROE / 1.0 0.1 584.9 6113. /
 H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
1
! Benzene oxidation
```

```
!
A1 + O \le C6H5O + H
                            2.20E+13 0.0 4530.0 ! CEC
A1 + OH \iff C6H5OH + H
                             1.30E+13 0.0 10600.0 ! CEC
!A1 - + O2 \iff C6H5O + O
                            2.10E+12 0.0 7470.0 ! LIN
A1 - + O2 \iff C6H5O + O
                            2.60E+13 0.00 6120.0 ! (Frank et al.)
1
!C6H5O <=> CO + C5H5
                            2.51E+11 0.0 43900.0 ! LIN
C6H5O <=> CO + C5H5
                            7.41E+11 0.0 43900.0 ! Frank et al.
C6H5O + H \le CO + C5H6
                              3.00E+13 0.0
                                             0.0 ! Est.
C6H5O + O <=> HCO + 2C2H2 + CO 3.00E+13 0.0
                                                 0.0 ! Est.
C6H5O + H (+M) \le C6H5OH (+M) 2.50E+14 0.0
                                                 0.0! (He et al.)
  LOW/1.00E+94 -21.84 13880.0/
                                         ! (HW, RRKM needs exam)
  TROE/0.043 304.2 60000. 5896.4/
 H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
I
C6H5OH + H \le C6H5O + H2
                               1.15E+14 0.0 12400.0 ! LIN
C6H5OH + O \iff C6H5O + OH
                                2.80E+13 0.0 7352.0 ! Brezinski
C6H5OH + OH <=> C6H5O + H2O 6.00E+12 0.0 0.0 ! LIN
C5H5 + H (+M) \le C5H6 (+M) = 1.00E + 14 = 0.0 = 0.0! (est. EBG)
   LOW/4.4E+80 -18.28 12994.0/
                                        ! (HW, RRKM)
  TROE/0.068 400.7 4135.8 5501.9/
 H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
C5H5 + O \le n-C4H5 + CO
                            1.00E+14 0.0 0.0 ! Brezinsky
C5H5 + OH \iff C5H4OH + H
                               5.00E+12 0.0
                                              0.0 ! Est.
C5H5 + HO2 \iff C5H5O + OH = 3.00E + 13 0.0
                                              0.0 ! Brezinsky
1
C5H6 + H \le C5H5 + H2
                             2.20E+08 1.77 3000.0 ! Brezinsky
                             1.80E+13 0.0 3080.0 ! Brezinsky
C5H6 + O \le C5H5 + OH
                              3.43E+09 1.18 -447.0 ! Brezinsky
C5H6 + OH \iff C5H5 + H2O
۱
C5H5O \le n-C4H5 + CO
                             2.50E+11 0.0 43900.0 ! Brezinsky
C5H5O + H <=> CH2O + 2C2H2 3.00E+13 0.0
                                               0.0 ! Est.
C5H5O + O \le CO2 + n-C4H5 = 3.00E+13 = 0.0
                                              0.0 ! Est.
۱
                             2.10E+13 0.0 48000.0 ! Brezinsky
C5H4OH \iff C5H4O + H
C5H4OH + H \le CH2O + 2C2H2 = 3.00E+13 = 0.0
                                                0.0 ! Est.
C5H4OH + O \le CO2 + n-C4H5 = 3.00E+13 = 0.0
                                               0.0 ! Est.
ļ
C5H4O \iff CO + C2H2 + C2H2
                               1.00E+15 0.0 78000.0 ! Brezinsky
C5H4O + O <=> CO2 + 2C2H2 3.00E+13 0.0 0.0 ! Est
1
aC3H5+CH3(+M) <=> C4H81(+M) 1.00E+14 -0.32 -262.3 ! TS5 300CM-1
            LOW / 3.51E+60 -12.97 6000.0

            TROE / 0.896 60000.0 1606.0 6118.4 /
  H2/2/H2O/6/CH4/2/CO/1.5/CO2/2/C2H6/3/AR/0.7/
C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/
! Reactions of 1-butene
!C4H81+H <=> C2H4+C2H5
                               17.6E+16 -1.05 6461.0 ! <=>(C3H6+H) TS5 0.1 atm*2
                               16.0E+21 -2.39 11180.0 ! <=>(C3H6+H) TS5 1 atm*2
C4H81+H <=> C2H4+C2H5
                               6.60E+24 -3.04 15610.0 ! <=>(C3H6+H) TS5 10 atm*2
!C4H81+H <=> C2H4+C2H5
C4H81+H <=> C3H6+CH3
                              32.0E+21 -2.39 11180.0 ! <=>(C4H81+H)*2
```

C4H81+H <=> C4H7+H2 6.50E+05 2.54 6756.0 !  $\leq (C3H8+H)/2$  TS5 k(a)  $C4H81+O \le nC3H7+HCO$ 3.30E+08 1.45 -402.0 ! Refit to Fontiin kadd C4H81+O <=> C4H7+OH 1.50E+13 0.00 5760.0 ! Fontijn duplicate C4H81+O <=> C4H7+OH 2.60E+13 0.00 4470.0 ! Fontijn duplicate 7.00E+02 2.66 527.0 ! <=>(C3H8+OH)/2 TS5 C4H81+OH <=> C4H7+H2O C4H81+O2 <=> C4H7+HO2 2.00E+13 0.00 50930.0 ! <=>(C3H8+O2)/2 TS5 !C4H81+HO2 <=> C4H7+H2O2 2.40E+04 2.55 16490.0 ! <=>(C3H8+HO2)/2 TS3 C4H81+HO2 <=> C4H7+H2O2 1.50E+11 0.00 14900.0 ! Walker 77 (/2) C4H81+CH3 <=> C4H7+CH4 4.50E-01 3.65 7153.0 ! <=>(C3H8+CH3)/2 TS5 k(c) ۱ ! Reactions of 1-buten-3-yl !C4H7 <=> C4H6+H 1.55E+56 -13.46 50860.0 ! HW 0.1 atm & C4H7 <=> C4H6+H 2.28E+52 -12.01 51230.0 ! HW 1 atm !C4H7 <=> C4H6+H 2.25E+44 -9.39 49150.0 ! HW 10 atm  $C4H7+H(+M) \le C4H81(+M)$ 3.60E+13 0.00 0.0 ! <=>(nC3H7+H) TS3 600 cm-1 LOW / 3.01E+48 -9.32 5833.6 TROE / 0.498 1314.0 1314.0 50000.0 / H2/2/H2O/6/CH4/2/CO/1.5/CO2/2/C2H6/3/AR/0.7/ C4H7+H <=> CH3+aC3H5 2.00E+21 -2.00 11000.0 ! Estimated  $C4H7+H \le C4H6+H2$ 1.80E+12 0.00  $0.0 ! \le (nC3H7+H) TS3$ C4H7+O2 <=> C4H6+HO2 1.00E+11 0.00 0.0 ! Estimated 0.0 ! <=>(nC3H7+HO2) TS3 C4H7+HO2 <=> CH2O+OH+aC3H5 2.40E+13 0.00 C4H7+HCO <=> C4H81+CO 6.00E+13 0.00 0.0 ! <=>(nC3H7+HCO) TS3 C4H7+CH3 <=> C4H6+CH4 1.10E+13 0.00 0.0 ! <=>(nC3H7+CH3)۱ ! Recombination reactions of C1 and C2 species !C2H3+C2H4 <=> C4H7 1.21E+05 2.33 3680.0 ! HW inf & !C2H3+C2H4 <=> C4H7 1.23E+35 -7.76 9930.0 ! HW 0.1 atm C2H3+C2H4 <=> C4H7 7.93E+38 -8.47 14220.0 ! HW 1 atm 2.99E+36 -7.40 15480.0 ! HW 10 atm !C2H3+C2H4 <=> C4H7 ! C2H3+C2H5(+M) <=> C4H81(+M) 1.50E+13 0.00 0.0 ! TS1 450cm-1 LOW / 1.55E+56 -11.79 8984.5 TROE / 0.198 2277.9 60000.0 5723.2 / H2/2/H2O/6/CH4/2/CO/1.5/CO2/2/C2H6/3/AR/0.7/ C2H4/3.0/ pC3H4/4.0/ C3H6/4.0/ C3H8/4.0/ ! kinf: -0.5 T power = CH3+C2H5, kinf(300K) = TS1 recommendation ! ko: scaled such that Pr(C2H5+C2H5) = Pr(CH3+C2H5) at (T,P), 500 cm-1 ! Fc: assumed equal to Fc(CH3+C2H5) ! PW Pitz and Westbrook ! HW Wang RRKM calcl ! CEC EC compilation ! TS1 Tsang, methane compilation ! TS3 Tsang, propane compilation ! TS4 Tsang, isobutane compilation ! TS5 Tsang, propene compilation ! TW Tsang, W. and Walker, J. A. J. Phys. Chem. 96:8378-8384 (1992). ! CW Cohen, N. and Westberg, K. R., Int. J. Chem. Kinet. 18:99 (1986) ! C Cohen, N. Int. J. Chem. Kinet. 23:397-417 (1991)

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! KP Kerr and Parsonage 1972 review
! Cvetanovic Cvetanovic, R.J. J. Phys. Chem. Ref. Data 16:261, 1987.
!
END
## **APPENDIX F: SAMPLE INPUT FILE FOR CHEMKIN ANALYSIS**

Following file is for a 200 K/mm temperature drop.

/ Automatically generated file for overnight Chemkin run
/ Premixed flame program
/ Quenching with thermal diffusion
/ Generated
/ Wed Jan 19 17:15:58 2005

**BURN** TGIV TDIF MULTI FLRT .11277 ! gm/cm\*\*2-sec PRES 1.0 ! atmospheres NPTS 30 NADP 50 TFIX 400. ATOL 1.E-9 RTOL 1.E-4 ATIM 1.E-5 RTIM 1.E-5 PRNT 1 TIME 100 5.0E-7 ! sec TIM2 200 1.0E-6 ! sec MOLE **NTOT 500** NADP 10 TDIF INTM CO 0.03 INTM HCO .1 INTM HO2 0.01 INTM O 0.01 INTM H2O2 0.01 INTM H 0.1 INTM H2 0.1 INTM OH 0.013 INTM CH2 .1 INTM CH .001 INTM CH2O .01 INTM CH3 .02 TEMP -5.0 298. TEMP -2 298.00 TEMP -0.5 298.00 TEMP -0.2 298.00 TEMP -0.08 298.00 TEMP -0.02 298.30 TEMP 0.01 300.10 TEMP 0.025 307.60 TEMP 0.0325 324.70 TEMP 0.0363 347.90

TEMP	0.0381	368.70
TEMP	0.04	400.00
ТЕМР	0.0409	421.00
TEMP	0.0419	446.60
TEMP	0.0428	477 10
TEMP	0.0437	512.90
TEMP	0.0437 0.0442	533.00
TEMP	0.0442	554.60
TEMD	0.0447	577 70
TEMP	0.0452	602.30
TEMD	0.0450	628.40
TEMP	0.0401	628.40
TEMP	0.0400	033.90
TEMP	0.04/5	715.00
TEMP	0.048	/46.30
TEMP	0.0484	//8.90
TEMP	0.0489	812.40
TEMP	0.0494	846.90
ТЕМР	0.0498	882.20
TEMP	0.0503	918.10
TEMP	0.0505	936.10
TEMP	0.0508	954.30
TEMP	0.051	972.50
TEMP	0.0512	990.80
TEMP	0.0515	1009.00
TEMP	0.0517	1027.00
TEMP	0.0522	1064.00
TEMP	0.0527	1100.00
TEMP	0.0531	1135.00
TEMP	0.0536	1169.00
TEMP	0.0541	1203.00
ТЕМР	0.0545	1236.00
TEMP	0.055	1267.00
TEMP	0.0555	1298.00
TEMP	0.0559	1327.00
TEMP	0.0564	1354.00
TEMP	0.0569	1380.00
TEMP	0.0573	1405.00
TEMP	0.0578	1428.00
TEMD	0.0578	1428.00
TEMP	0.0585	1471.00
TEMD	0.0507	14/1.00
TEMD	0.0592	1490.00
TEMP	0.0397	1508.00
TEMP	0.0002	1525.00
TEMP	0.0606	1540.00
TEMP	0.0611	1555.00
TEMP	0.0616	1568.00
TEMP	0.062	1581.00
TEMP	0.0625	1592.00
ТЕМР	0.063	1603.00
TEMP	0.0634	1613.00
TEMP	0.0644	1632.00
TEMP	0.0653	1648.00
TEMP	0.0662	1662.00
TEMP	0.0672	1676.00
TEMP	0.0681	1688.00
TEMP	0.07	1709.00

TEMP	0.0737	1744.00
TEMP	0.0775	1774.00
TEMP	0.085	1822.00
TEMP	0.0925	1861.00
TEMP	0.1	1893.00
TEMP	0.1187	1953.00
TEMP	0.1375	1998.00
TEMP	0.175	2059
TEMP	0.25 190	9
TEMP	0.4 1609	
TEMP	0.7 1009	
TEMP	1	409
TEMP	2	300
TEMP	3	300

/ Starting Calculation for slope of 2000. REAC C3H8 0.0134198 REAC H2 0.197132 REAC O2 0.163579 REAC N2 0.62587 XSTR -0.5 XCEN 0.1 XEND 2.0 ! cm WMIX .1 ! cm GRAD 0.9 CURV 0.9 **CNTN** END / / This is the second continuation for 2000. The mesh adaptation is more / stringent, and th computational comain is expanded. Yet another / continuation will follow after this one. / GRAD 0.5 CURV 0.5 XSTR -0.5 XEND 3.0 CNTN END / / This is the third and final continuation for 2000. The mesh adaptation / is more stringent, and th computational domain is again expanded. / FINAL ANSWER BELOW!! GRAD 0.35 CURV 0.35 XEND 3.0 XSTR -.5 **CNTN** END