DETERMINATION OF FLAME CHARACTERISTICS IN A LOW SWIRL BURNER AT GAS TURBINE CONDITIONS THROUGH REACTION ZONE IMAGING

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X_f Flame standoff distance

CHAPTER 1

EXPERIMENTAL METHODS AND CONSIDERATIONS

The current chapter details the facilities and apparatus used to study the flame characteristics in a Low Swirl Burner. The selection and implementation of diagnostic techniques used in this study are explained, as are data analysis methods used to process the acquired data.

1.1 LSB configuration

Two configurations of the Low Swirl Burner were tested for this study. There are referred to in what follows as Configurations A and B. Each configuration is built around a swirler with an outer diameter, d_s of 38 mm (1.5 in). Other key dimensions of the swirlers tested for this work are presented in Table **??**.

Initial testing aimed at velocity field mapping and flame imaging is conducted on Configuration A, while Configuration B is used for a later series of tests aimed at visualizing the flame structure. The design of these two configurations is discussed in further detail in what follows.

1.1.1 Configuration A

In this configuration, the reactants reach the swirler through a converging nozzle that decreases linearly in diameter from from the inlet diameter of 102 mm (4 in) to the outer diameter of the swirler, 38 mm (1.5 in). The swirler leads to a constant area nozzle, and is located one diameter upstream of an abrupt area change. At the area change, the reactants expand from the 38 mm (1.5 in) diameter nozzle into a 115 mm (4.5 in) diameter combustion zone. The expansion ratio is chosen so as to avoid confinement effects on the centerline flame flow field.[1]

Table 1.1: *The dimensions of the swirlers used and the respective perforated plates are presented. Each swirler is referred to by its vane angle (as in "$S_{37°}$").*

Geometric parameter	Swirler	
	$S_{37°}$	$S_{45°}$
Swirler data		
Outer diameter, d_s, mm	38	38
Diameter ratio, $\frac{d_i}{d_s}$	0.66	0.66
Vane angle, α	37°	45°
Theoretical Swirl Number, S	0.48	0.64
Perforated plate data		
Open area, mm^2	155.97	156.98
Blockage, %	71.54	71.36
Plate thickness, mm	1.27	1.27
Hole pattern	1 - 8 - 16	1 - 8 - 16
Hole location (dia), mm	0 - 10.2 - 19.1	0 - 10.2 - 19.1
Hole diameter, mm	2.79 - 2.79 - 2.84	2.82 - 2.82 - 2.83

The main combustion zone begins at the dump plane and is enclosed by a GE 214 quartz tube. The quartz tube is 300 mm (12 in) long and 115 mm (4.5 in) in diameter. The thickness of the quartz tube is 2.5 mm (0.1 in). Configuration A is illustrated in Figure FIXME.

1.1.2 Configuration B

In configuration B, the reactants reach the swirler through two separate streams. The core stream passes through a layer of ball bearings before passing through a smoothly contoured nozzle with a high contraction ratio. The annular stream passes directly through a smoothly contoured nozzle. The contractions are designed to inhibit the formation of thick boundary layers. The core stream passes through the central section of the swirler, while the annular stream picks up swirl by passing through the vanes of the swirler.

The swirler is located upstream of a constant area nozzle which is FIXME in

length. The reactants then expand into the combustion zone. ³⁷

Unlike in Configuration A, there is no dump plane or quartz tube to provide ³⁸ confinement to the combustion zone. The walls of the pressure vessel are insulated ³⁹ from the combustion zone by a co-flow of cold air. Further, in this configuration, ⁴⁰ the annular flow is separately controlled from the central flow, which allows one to ⁴¹ control the mass flow split directly, if necessary. Finally, this configuration allows ⁴² for adjusting the level of turbulence present in the inlet flow by use of a turbulence ⁴³ generator located upstream in the plenum chamber. ⁴⁴

The details of Configuration B are shown in Figure FIXME. ⁴⁵

1.2 High Pressure Test Rig ⁴⁶

Each of the two configurations is housed in a separate high pressure testing rig with ⁴⁷ optical access to study the flame. These rigs consist of an air and fuel supply system, ⁴⁸ a pressure vessel with adequate optical access and an exhaust system. The details of ⁴⁹ each rig are discussed in the following sub-sections. ⁵⁰

1.2.1 Test Rig A ⁵¹

Preliminary experiments involving velocity field mapping and flame imaging are con- ⁵² ducted in Test Rig A, shown in Figure FIXME. Preheated air at about 500 K is ⁵³ drawn from external tanks and metered through an orifice flow meter. The air enters ⁵⁴ the inlet nozzle of the LSB through a 1.8 m (6 ft) long, 102 mm (4 in) diameter ⁵⁵ straight pipe section. Fuel (natural gas) is metered using another orifice flow meter ⁵⁶ and injected at the head of the straight pipe section. The straight pipe section allows ⁵⁷ for the flow to be fully developed, and fully premixed before the reactants enter the ⁵⁸ burner. ⁵⁹

The combustor pressure and temperature are measured at the head of the inlet ⁶⁰ nozzle by a pressure transducer and a thermocouple respectively. In addition, the ⁶¹

upstream pressure and the pressure differential are measured at the air and fuel ₆₂ orifice flow meters. For the preheated air stream, the upstream temperature is also ₆₃ measured. The measurements are used to calculate the four primary flow parameters ₆₄ (combustor pressure, preheat temperature, reference velocity and equivalence ratio) ₆₅ for the LSB in real time. All measurements are monitored and recorded during the ₆₆ course of the experiment by a LabView VI. ₆₇

The pressure vessel enclosing the combustor is designed to withstand pressures of ₆₈ up to 30 atm and is insulated from the combustor by a ceramic liner. Cooling for the ₆₉ pressure vessel and the quartz tube is provided by a flow of cold air introduced at ₇₀ the head of the pressure vessel. Optical access to the combustor is provided through ₇₁ four 25 mm (1 in) thick, 150 mm (6 in) × 75 mm (3 in) quartz windows located 90° ₇₂ apart azimuthally. The view ports allow the combustor to be imaged from the dump ₇₃ plane to an axial distance of 150 mm (6 in) downstream. ₇₄

The exhaust from the combustor is cooled by circulating cold water through a ₇₅ water jacket enclosing the exhaust pipe section. The length of the exhaust pipe ₇₆ section is about FIXME. The exhaust pipe section terminates in an orifice plug to ₇₇ provide the back pressure to the combustion chamber. Different diameter orifices ₇₈ are used for each reference velocity condition to be tested. The exiting products are ₇₉ finally released to the building exhaust system. ₈₀

1.2.2 Test Rig B ₈₁

A schematic of Test Rig B is shown in Figure FIXME. Both test rigs share the same ₈₂ upstream supply of preheated air, cold air and natural gas. The preheated air splits ₈₃ into two separate streams a short distance after mixing with the natural gas fuel. ₈₄ Orifice flow meters are used to meter the air and fuel flows prior to mixing. Further, ₈₅ each reactant stream is individually metered by separate orifice flow meters. This ₈₆ builds redundancy in the system, offering a double-check of all readings and verifies ₈₇

that there are no leaks in the flow system. Each orifice flow meter is equipped with a   88
thermocouple, an upstream pressure transducer and a differential pressure transducer.   89
The cooling air for the co-flow is not metered. All measurements are monitored and   90
recorded by a LabView VI.   91

The pressure vessel is rated for pressures in excess of 30 atm and is insulated from   92
the combustor by a flow of cold air. The cold air enters the pressure vessel through   93
two inlet ports and passes through a layer of steel ball bearings which renders the   94
flow uniform spatially. The pressure vessel has four viewports located 90° apart for   95
optical access. Each viewport is covered by a 25 mm (1 in) thick, 178 mm (7 in) ×   96
50 mm (2 in) quartz window. The inlet of the LSB is located approximately halfway   97
between the top and bottom edges of the window.   98

Similar to Test Rig A, the exhaust section is cooled by circulating cold water   99
through an enclosing water jacket. An adjustable gate valve on the exhaust line   100
provides the back pressure necessary to pressurize the combustor. The products are   101
vented into the building exhaust system.   102

1.3 Diagnostics   103

1.3.1 Laser Doppler Velocimetry   104

The velocity field of the LSB is mapped using a TSI 3-component LDV system.   105
Three wavelengths (514 nm, 488 nm and 476 nm) are separated from the output of a   106
5 W Argon ion laser by an FBL-3 multicolor beam generator. The individual beams   107
are split into two coherent beams which are then focused to intersect and produce   108
interference fringes within an ellipsoidal measurement volume with dimensions of the   109
order of 100 μm. For this purpose, two transceiver probes are mounted 90° apart   110
about the axis of the LSB. One transceiver probe focuses the 514 nm and 488 nm   111
beams in planes perpendicular to each other, while the second probe focuses the 476   112
nm beams orthogonal to the other two beams. Particles in the flow field crossing the   113

interference fringes scatter the laser light elastically and produce a sinusoidal signal 114

whose frequency is proportional to the velocity of the particle. The transceiver probes 115

collect this scattered light and each wavelength is detected separately by a PDM- 116

1000-3 three-channel photodetector module. The output from the photodetector is 117

processed by an FSA-3500-3 signal processor. The resulting three components of the 118

particle/flow velocity are recorded by the FlowSizer software. 119

Since the airflow is very sparsely populated by particles, the flow needs to be 120

artificially seeded to facilitate LDV measurements in a reasonable amount of time. 121

The seeding particles to be used and their mean diameter are decided by the charac- 122

teristics of the flow to be imaged.[2] Since the LSB flow field is a reacting one, the 123

particles need to have high melting points. Further, the particles need to be small 124

enough to follow the flow closely and large enough or reflective enough to scatter light 125

efficiently in the measurement volume. Based on these requirements, commercially 126

available alumina particles with a mean particle diameter of 5 μm were chosen for this 127

study. In order to uniformly seed the flow, a novel seeding generator was designed as 128

described in Appendix A. The seeding particles were introduced slightly upstream of 129

the 1.8 m (6 ft) long straight pipe section in Test Rig A. 130

LDV data is only acquired at atmospheric pressure conditions. At high pressure 131

conditions, the reacting LSB flow field produces sharp refractive index gradients that 132

rapidly shift in the turbulent flow field. This causes strong beam steering effects 133

making it very difficult for the laser beams to reliably intersect within such a small 134

measurement volume. The long distance traveled by the beams in the test rig further 135

exacerbated this problem, making LDV data nearly impossible to acquire at such 136

conditions. 137

The LSB flame is imaged using one of two 16-bit intensified CCD cameras — PI 139
Acton 1024×256 or 512×512 pixels — with a 28 mm f/2.8 camera lens. CH* chemi- 140
luminescence is filtered using a bandpass filter centered on 430 nm with a FWHM 141
of 10 nm. At each operating condition, 100 instantaneous images are acquired with 142
an exposure of 1 ms. An additional 100 instantaneous images are acquired with no 143
flame and averaged to yield the background for correcting the flame images. 144

CH* chemiluminescence has several advantages over flame chemiluminescence 145
from other radicals such as OH*, C_2*, etc. First, the CH* emission occurs around 146
430 nm and is not affected by blackbody radiation from the walls of the combustor. 147
C_2*, on the other hand, emits around 514 nm and is significantly affected by this 148
issue. Second, the intensity of the chemiluminescence from CH* is known to scale 149
well with heat release in the combustor[3], unlike C_2*. Third, the emitted light can 150
be gathered with high quantum efficiency by the intensified CCD cameras used for 151
this study. The quantum efficiency of the 18 mm Gen III HB filmless intensifier used 152
by the 512×512 camera is about 45% at 430 nm, compared to about 10% at 310 nm, 153
where OH* chemiluminescence peaks. 154

1.3.2.1 Image Processing

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The flame chemiluminescence images acquired are background-corrected and aver- 157
aged. The resulting mean is the line-of-sight integrated, time-averaged image of the 158
flame. Strictly speaking, this is not the same as a real average obtained from a long 159
exposure image. The instantaneous images are obtained through a periodic sampling 160
process and hence, are prone to statistical errors and aliasing. However, the behaviour 161
of the flame can be assumed to be sufficiently random, and the mean obtained is ade- 162
quately representative of the true average. Figure FIXME shows a typical mean CH* 163

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chemiluminescence image prepared in this manner. 164

Even when background-corrected, the walls of the combustor are not at zero in- 165
tensity in the average chemiluminescence image. This is particularly noticeable near 166
the dump plane where there is no flame present and yet the walls are clearly illumi- 167
nated. The source of this illumination is mostly scattered chemiluminescence from the 168
flame itself, and to a lesser degree, blackbody radiation from the heated walls. The 169
averaged chemiluminescence image allows us to measure the flame standoff distance 170
by following the intensity profile along the centerline of the combustor. The inten- 171
sity profile rises sharply when passing the flame standoff location. Thus, the flame 172
standoff location can be ascertained by finding the inflection point in the intensity 173
profile. 174

The profile of the average chemiluminescence intensity along the centerline of the 175
sample case from Figure FIXME is shown in Figure FIXME, showing the flame stand- 176
off distance. The distance from the dump plane, measured in number of pixels on 177
the image and scaled by the appropriate magnification factor yields the flame stand- 178
off distance, X_f. The determination of the flame standoff location by this method 179
provides a suitable and deterministic means to locating the leading edge of the flame 180
front. 181

The average image can be processed further to yield more spatially resolved in- 182
formation about the flame brush. Under the reasonable assumption that the average 183
LSB flame is axially symmetric about the centerline of the combustor, a tomographic 184
deconvolution technique called the Abel deconvolution[4] can be used to convert the 185
line-of-sight integrated image to a radial map of chemiluminescence intensity. In 186
effect, this shows the shape and structure of the average flame brush. The Abel 187
deconvolution of the sample data from Figure FIXME is shown in Figure FIXME. 188

The Abel-deconvoluted image provides an relatively easy means to determining 189
the angle of the flame brush. A straight line joining two points located at the center 190

of the flame brush intersects the axis of the combustor at this angle. The angle of the flame is denoted by θ_f.

Using the Abel deconvolution to study the flame brush suffers from two main drawbacks. First, the system of equations describing the Abel deconvolution is only valid as long as the entirety of the flame is visible. This is only satisfied in the initial region of the LSB where the diameter of the flame brush is smaller than the height of the optical viewport. At further downstream locations, the flame is not imaged in its entirety. This causes the spurious bright regions near the top of the window in Figure FIXME. The second limitation of the Abel deconvolution technique stems from the high incidence of errors along the centerline (where $r \to 0$). Due to this, any study of the flame brush thickness at the flame stabilization point — a metric of considerable importance — is all but impossible using this tomographic technique.

1.3.3 CH Planar Laser Induced Fluorescence

The CH PLIF setup uses the frequency-doubled output of a Light Age PAL 101 alexandrite laser tuned to $\lambda \approx 387.2$ nm to pump the R-bandhead of the CH $B^2\Sigma^- \leftarrow X^2\Pi$ (0,0) system. This populates the $A^2\Delta$ state through fast electronic energy transfer from the $B^2\Sigma^-$ state. The resulting broadband fluorescence observed between $\lambda = 420$–440 nm is due to the $A^2\Delta \to X^2\Pi$ (1,1), $A^2\Delta \to X^2\Pi$ (0,0) and $B^2\Sigma^- \to X^2\Pi$ (0,1) bands. The CH PLIF signal is collected using an intensified PI Acton $512{\times}512$ camera equipped with an 18 mm Gen III HB filmless intensifier with a quantum efficiency of about 45% in the 420–440 nm range. Elastic scattering from the laser beam is attenuated by a 3 mm thick GG 420 Schott Glass filter.

1.3.3.1 Laser Wavelength Calibration

The output of the PAL 101 alexandrite laser is controlled using a micrometer-coupled birefringent tuning mechanism. The output wavelength of the laser varies linearly

with the micrometer reading. Initially, the manufacturer-supplied calibration for the 217
micrometer was found to be inaccurate. This required the recalibration of the laser 218
in order to know the slope and offset of the calibration curve. 219

An Ocean Optics HR 2000 spectrometer is used to get the true wavelength of the 220
laser output. The spectrometer is pre-calibrated using 50 wavelengths in the 400–850 221
nm range from output of an Neon discharge lamp source. The spectrometer is also 222
intensity corrected over this range using a black body source. The estimated error in 223
the resolution of the device is about 0.1 nm (1 Å). 224

The laser micrometer was traversed from 0.600 in to 0.626 in and back in steps 225
of 0.001 in. The calibration was performed using the fundamental wavelength of 226
the laser. Spectra were recorded at these conditions, integrated over 512 ms, and 227
averaged over 10 acquisitions. Each acquired spectrum was modeled as a Gaussian 228
and the location of the center wavelength was noted. The variation of the wavelength 229
is verified to be linear against the micrometer setting and the correct calibration 230
equation is obtained by doing a linear curve fit of the data. The results are shown in 231
Figure FIXME. 232

1.3.3.2 Excitation scan 233
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An excitation scan is performed by tuning the output of the laser from $\lambda = 387.077$ 235
nm to 387.260 nm. This serves two purposes. First, it locates the optimal wavelength 236
to excite the CH radicals that results in the highest fluorescence yield. Second, 237
the variation of the signal intensity can be compared with simulated profiles from 238
LIFBASE and our calculation of the laser linewidth can be validated. 239

In order to do this, the CH PLIF imaging system, consisting of the alexandrite 240
laser and the intensified PI Acton 512×512 camera is used to image a premixed, sto- 241
ichiometric, laminar methane-air flame. The laminar flame is stabilized on a Bunsen 242
burner with an inner diameter of 10.16 mm (0.4 in). The alexandrite laser is operated 243

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at 10 Hz, with a power of 16 mJ/pulse. The second harmonic beam is refracted into 244
a sheet about 25 mm tall, with a thickness on the order of 100 μm passing through 245
the center of the flame. The edges of the sheet are blocked by razor blades. 246

The induced fluorescence is imaged perpendicularly by the intensified camera using 247
an 85 mm f/1.8 Nikon AF Nikkor lens and the intensifier is gated over 300 ns. 100 248
instantaneous images are acquired for each case. The resolution of the imaging system 249
is approximately 62 μm per pixel. 250

Figure FIXME shows a sample CH PLIF image from this dataset. The images 251
are background-corrected and the signal statistics are measured at the midpoint of 252
the flame. 253

The mean of the CH PLIF signal is compared with the LIFBASE-simulated profile 254
of CH excitation LIF output. The two signals are normalized by their individual 255
maxima and plotted in Figure FIXME. The profiles agree extremely well, validating 256
our calibration of the laser output and our calculation of the laser linewidth. The 257
optimal excitation wavelength is found to be about 387.2 nm. 258

1.3.3.3 Linearity test

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The next step is to estimate the variation of the LIF signal as a function of the 261
operating conditions. However, this function depends on which LIF regime we operate 262
in. Hence, it is imperative that we verify the regime of operation before attempting 263
to model the CH PLIF signal. 264

Under the assumption that the CH ground state population is not depleted by 265
excitation or laser-induced chemical reactions, the LIF signal is linearly proportional 266
to the laser intensity in the weak excitation limit. However, as the laser intensity 267
is increased further, the LIF output is observed to saturate and plateau. This is 268
called the strong excitation limit/saturation regime. In the weak excitation limit, the 269
signal is a function of CH concentration and the rate of collisional quenching of the 270

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excited CH radicals. In the strong excitation limit, the signal depends only on the CH concentration is unaffected by the quenching of the excited CH species.

It is difficult to ensure that the CH system is saturated spatially, temporally and spectrally at the same time. Further, operating with high laser intensities may bleach the energy levels being excited by inducing chemical reactions that destroy the excited CH radicals. Hence, it is preferred to operate in the linear regime.

For this experiment, the laser beam is directed at a steady, laminar, methane-air, Bunsen flame operating at a slightly rich stoichiometry. The 1 mm diameter beam is passed through an aperture, but no optics are used to refract the beam otherwise. Varying the intensity of the laser beam by changing the flash lamp voltage or the Q-switch timing is not preferred as either would alter the pulse-width of the beam. Instead, quartz disks and blocks are introduced into the beam to produce an intensity loss through reflection, scattering and absorption.

The flame is imaged with the PI Acton 512×512 intensified camera equipped with a 50 mm, f/1.8 AF Nikkor lens and a 3 mm thick GG 420 filter. The resolution of the set up was measured to be about 44 μm/pixel. The laser power was varied from 10 mJ/pulse to 0.5 mJ/pulse in the manner described earlier. The LIF signal image was recorded over 150 accumulations. The corresponding laser scattering image was also recorded at each power for better estimating the background. The flame chemiluminescence was also recorded for the same purpose.

The average signal per pixel is plotted in arbitrary units against the laser intensity in Figure FIXME. The results indicate that the linearity of the LIF signal is valid for all laser intensities under 1 J/cm^2.

CHAPTER 2

CH PLIF SIGNAL MODELING AND VALIDATION

2.1 Fluorescence Signal Intensity

As described in Chapter FIXME 2, the excitation scheme used in this study produces fluorescence through a three-step process. First, the CH radicals in the ground state $X^2\Pi, v = 0$ are excited by the incident radiation to the second electronically excited state $B^2\Sigma^-, v = 0$. This excitation occurs near the R-bandhead and targets the ground state CH radicals present in the rotational energy levels, $N = 5$ through 9. The upper electronic state $B^2\Sigma^-, v = 0$ is nearly degenerate with the $A^2\Delta, v = 1$ energy level. This leads to the population of the $A^2\Delta, v = 0, 1$ energy levels due to collisional energy transfer. The resulting fluorescence collected is primarily the result of three spontaneous transitions — $A \to X(1,1)$, $A \to X(0,0)$ and $B \to X(0,1)$. These transitions are shown in Figure FIXME.

The primary goal of this exercise of modeling the CH fluorescence signal intensity is to gage the feasibility of using CH PLIF to study various premixed flames, rather than to quantitatively calculate the amount of CH present in the flames. As such, we are more interested in the order of magnitude of the PLIF signal, rather than the absolute value of it.

The intensity of the CH fluorescence signal may be written as a function of the amount of CH radicals present in the excited state and the probability of spontaneous emission from said state. Symbolically, this may be written as shown in Equation B.1.

$$S = nVA \tag{2.1}$$

In Equation B.1, S is the total number of photons emitted per unit time, n is the number of excited CH radicals in a unit volume, V is the volume from which the signal is observed. The Einstein coefficient for spontaneous emission, A represents the probability of spontaneous emission between the two involved energy states. The predicted signal intensity represents the total number of photons emitted in all directions. In reality, only a fraction of these emitted photons will be recorded by the collection system. This fraction is a function of the experimental setup and depends on the collection angle, the efficiency of the optics and the detector used to record the signal. This fraction is left out because our objective is only to predict the relative variation in the signal between various premixed flames.

This formulation of the signal intensity implicitly makes the following assumptions.

1. The fluorescence emission is predicted at steady state.

2. The collection volume is optically thin and an emitted photon is not reabsorbed within the flame itself. This is a reasonable assumption to make, since the flame thickness and the thickness of the laser sheet are both typically quite small.

As described earlier, an accurate model of the CH system should involve five energy levels — $X(0)$, $B(0)$, $A(1)$, $A(0)$, and $X(1)$[1]. Such a model would also have to account for collisional transfers between each of these levels, in addition to spontaneous and stimulated transitions. The mathematical solution quickly becomes complicated and tedious. Further, it would involve several rate coefficients that have not been measured in experiments done so far.

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[1]In this notation, the letter represents the electronic energy level and the number in the parentheses represents the vibrational quantum number of the energy level

CHAPTER 3

LSB FLAME CHARACTERISTICS

In Chapter FIXME 2, we introduced the salient features of the Low Swirl Burner (LSB) flow field and discussed the mechanisms by which the LSB flame is stabilized. Further, various characteristics of the LSB flame that can be measured from flame images were outlined. To recapitulate, these are the flame location, flame shape and the flame structure. The first two are quantified by the flame standoff distance, X_f, and the flame angle, θ_f, respectively.

In the same chapter, we introduced the four flow parameters that describe an operating condition for the LSB — the combustor pressure, p, the preheat temperature, T, the mass-averaged inlet velocity (also called the reference velocity, U_0), and the equivalence ratio of the premixed reactants, ϕ. We further introduced a geometric parameter — the angle of the vanes of the swirler, α, which affects the amount of swirl present in the flow field.

The LSB flame was studied over a range of operating conditions, and the effect of flow and geometric parameters on the reacting flow field were investigated. The results of these investigations are presented in this chapter.

3.1 Effect of reference velocity

In typical gas turbine applications, varying the loading on the engine does not affect the reference velocity. However, since the reference velocity is a design parameter, the effect it has on the flame characteristics has implications for the design of future LSB-based gas turbine engines.

One of the key objectives of this thesis is to investigate how the LSB flame stabilization operates at high pressure conditions. The simple model described in Chapter

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FIXME 2 predicts a self-similar flow field for the LSB at all reference velocities. This implies that the reference velocity will have no discernible impact on the flame stand-off distance. This result is desirable for gas turbine designers, since the flame location and shape can be assumed to be constant. Limited testing conducted in published works confirmed this behavior at atmospheric pressure conditions with no preheat.

In order to verify the validity of this model at high pressure conditions in the presence of substantial preheat, the LSB was operated at a pressure of 6 atm over a range of reference velocities from 10 m/s to 40 m/s. For these tests, the $S_{37°}$ swirler was used. In a parallel series of tests, the $S_{45°}$ swirler was tested at a pressure of 3 atm at a reference velocities of 40 and 80 m/s. The location of the flame was measured from CH* chemiluminescence images, and the results are presented in Figure FIXME.

There is essentially no systematic variation in the flame standoff distance or the flame angle for the low velocity, $S_{37°}$ tests. Based on the model, this can be interpreted as the increase in reference velocity producing a concomitant increase in the turbulent flame speed at the flame stabilization location, negating any change in the flame's location. In other words, the flow field appears to retain its self-similarity, even at elevated pressures and temperatures.

When the $S_{45°}$ swirler was tested at higher reference velocities, however, the flame location shifted downstream sharply. This indicates potential limitations to the simple flame stabilization model that may not predict the behavior of the LSB flame at elevated pressures and temperatures, particularly at high reference velocities.

A possibe cause of this limitation can be explored by considering the effect of increased reference velocity on the turbulent combustion regime in which the LSB combustor operates. Previous studies have primarily operated the LSB in the flamelet regime where the modified Damköhler model predicts the behavior of the turbulent flame speed with reasonable fidelity. At elevated pressures, both the laminar flame speed of the reactants, S_L and the flame thickness, δ_f are diminished. This places

the operating regime higher and more to the right on a Borghi diagram, as shown in ³⁸⁸ Figure FIXME. While increasing the reference velocity did not affect the turbulent ³⁸⁹ combustion regime at lower pressures in a flamelet combustion regime, at elevated ³⁹⁰ pressures the flame may be transitioning into the thin reaction zone regime. This ³⁹¹ transition would cause a reduction in S_T/S_L, or at least a lesser increase, and the ³⁹² turbulent flame speed would no longer be expected to increase in step with U_0 and ³⁹³ the increased levels of turbulence. This would explain the the observed downstream ³⁹⁴ shift of the high pressure LSB flame at high reference velocities. ³⁹⁵

3.2 Effect of preheat temperature ³⁹⁶

The preheat temperature of the reactants is a key flow parameter, especially for gas ³⁹⁷ turbine combustors. In general, the rates of most chemical reactions in the flame zone ³⁹⁸ are highly sensitive to the temperature of the reactants. For the LSB in particular, ³⁹⁹ the temperature of the incoming flow directly affects its viscosity and consequently, ⁴⁰⁰ the velocity field in the flame stabilization region. Thus, studying the effect of the ⁴⁰¹ preheat temperature on the LSB flame and flow field is important. ⁴⁰²

In order to explore this in greater detail, the velocity field of the combustor was ⁴⁰³ mapped using Laser Doppler Velocimetry (LDV). The conditions were chosen to study ⁴⁰⁴ the effect of increasing the preheat temperature on both reacting and non-reacting ⁴⁰⁵ LSB flow fields. Further, the study includes both low and high reference velocity cases. ⁴⁰⁶ The relevant flow parameters relating to these tests are presented in Table FIXME. ⁴⁰⁷ All LDV tests were limited to atmospheric pressure conditions. Implementing the ⁴⁰⁸ LDV technique at elevated pressures proved difficult due to beam steering issues, ⁴⁰⁹ coupled with impractical turn-around times between the successive runs that would ⁴¹⁰ be required to obtain sufficent LDV data points for analysis. ⁴¹¹

The normalized centerline mean and rms axial velocity profiles for the three cases ⁴¹² are presented in Figure FIXME. The abscissa represents the distance from a point ⁴¹³

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called the virtual origin, X_0. The virtual origin is defined as the imaginary location $_{414}$ where the extrapolated linear axial velocity profile reaches the reference velocity in $_{415}$ magnitude. The extrapolation is indicated in Figure FIXME by a dashed line. $_{416}$

As noted in Chapter FIXME 2, previous studies[5] reported that mean axial $_{417}$ stretch — the normalized slope of the linear decay of axial velocity — at the in- $_{418}$ let of the combustor was self-similar, regardless of the Reynolds number, Re of the $_{419}$ operating condition. Further, it was reported that the velocity decay was steeper for $_{420}$ reacting cases compared to non-reacting cases. $_{421}$

The results presented in Figure FIXME however, show that even though Cases 1 $_{422}$ and 2 have similar Re, their mean velocity profiles have very different slopes. Further, $_{423}$ the reacting and non-reacting cases (both at preheated conditions) have similarly $_{424}$ steep slopes. This indicates that the mean axial stretch in the near field of the LSB $_{425}$ flow field is a stronger function of the preheat temperature than Re. The presence $_{426}$ of preheat results in increased viscosity that enhances the momentum transport in $_{427}$ the radial direction. This causes the velocity decay to be steep for preheated cases, $_{428}$ compared to cases without preheat. $_{429}$

Assuming that S_T is constant, these results suggest that at higher preheat tem- $_{430}$ peratures, the flame would stabilize closer to the dump plane because of the faster $_{431}$ velocity decay and reduced local flow velocities. In fact, a faster velocity decay would $_{432}$ produce greater u' values and increase S_T, further causing the flame location to shift $_{433}$ upstream. Furthermore, in view of the steep velocity profile, it may be anticipated $_{434}$ that any changes in the stabilization location caused by perturbations in the local $_{435}$ flow field (and hence, the local turbulent flame propagation velocity) are likely to be $_{436}$ of diminished magnitude in the presence of preheat. All of this leads to an intuitive $_{437}$ result — the LSB flame behaves more stably at high preheat conditions. $_{438}$

3.3 Effect of swirler vane angle

As described in Chapter FIXME 3, the LSB swirlers tested for this study are designed to have the same mass flow splits. The $S_{45°}$ swirler has a higher vane angle, resulting in greater blockage to the flow passing through the annular section. In order to compensate for this, the perforated plate covering the central section has slightly smaller holes. The net effect retains the same mass flow split as in the $S_{37°}$ swirler.

Chapter FIXME 2 describes how the swirler vane angle relates to the amount of swirl imparted to the incoming flow. According to Equation FIXME, a swirler with a higher vane angle will produce greater swirl in the reactants. Previous work in swirl combustion[6, 7] has pointed out that increased swirl shortens the flame by enhancing the swirl-induced radial pressure gradients. The data acquired in the present investigation is in agreement with this observation. Operated at identical inlet conditions, the $S_{45°}$ swirler stabilizes a flame closer to the dump plane and with a larger flame angle compared to the $S_{37°}$ swirler.

This result highlights an interesting trade-off for the designers of LSB-based gas turbine engines. The $S_{45°}$ flame is located further upstream and has a more concen- trated region of heat release. This enhances the strength of the toroidal recirculation zone near the dump plane, which may be powerful enough under certain conditions (as we shall see in Section 3.4) to even cause the flame to attach itself to the lip of the inlet. All of this means that the $S_{45°}$ flame is more stable and will resist pertur- bations in the incoming flow better than the $S_{37°}$ flame. However, the presence of a strong recirculation zone in the flow field of the $S_{45°}$ swirler will entrain more hot products and retain them longer near the zone of heat release. This is a recipe for the production of thermal NO_x. While no emission measurements were made as part of this study, it may be reasonably anticipated that the NO_x performance of the $S_{45°}$ swirler will be degraded compared to the $S_{37°}$ swirler. The trade-off for gas turbine

engine designers is thus between flame stability and emissions performance. ₄₆₅

3.4 Effect of equivalence ratio ₄₆₆

The LSB is primarily intended for fuel-lean operation in order to utilize its low NO_x ₄₆₇
emission performance. As a result, most of the testing was done as close as possible ₄₆₈
to a target ϕ of 0.56. Limited testing was carried out at 12 atm for two off-target ₄₆₉
conditions: a slightly richer ($\phi \approx 0.58$) and a slightly leaner ($\phi \approx 0.53$) mixture, in ₄₇₀
order to explore the sensitivity of the LSB flame to limited changes in equivalence ₄₇₁
ratio. The $S_{45°}$ swirler was used for these tests. The corresponding averaged and ₄₇₂
Abel-deconvoluted flame images are presented in Figure FIXME. ₄₇₃

Two characteristics of the flame are immediately obvious from these images. First, ₄₇₄
the zone of heat release, marked by the region from which CH* chemiluminescence ₄₇₅
is observed, is increasingly compact at fuel-rich conditions. Virtually all other flame ₄₇₆
images acquired at a leaner condition show a long flame, with the heat release dis- ₄₇₇
tributed over the entire visible area of the combustor. The compactness of the heat ₄₇₈
release zone indicates potentially poor NO_x performance at these conditions. ₄₇₉

Second, the fuel-rich flame brush can be observed to wrap around and anchor itself ₄₈₀
on the dump plane. This is particularly observable in the Abel-deconvoluted image. ₄₈₁
The attached region is not as bright as the rest of the flame brush, indicating that ₄₈₂
the flame may be attaching itself intermittently. This intermittent behavior can be ₄₈₃
confirmed from the instantaneous images where it is visible on some of the acquired ₄₈₄
images, but not others. This behavior was alluded to in Section 3.3 as being the ₄₈₅
result of the enhanced toroidal recirculation zone produced by this swirler. Thus, the ₄₈₆
intermittent attachment of the flame to the inlet indicates the increased importance ₄₈₇
of the toroidal recirculation zone in stabilizing the flame. ₄₈₈

It should be noted that the reliance on a toroidal recirculation zone to anchor ₄₈₉
the flame to the inlet is one of the primary flame stabilization mechanisms used by ₄₉₀

traditional swirl combustors. Thus, LSB swirlers with high vane angles tend to behave like traditional swirl combustors at fuel-rich conditions.

3.5 Effect of combustor pressure

In many gas turbine engines, the combustor pressure varies directly with the loading of the engine. Like the preheat temperature, the combustor pressure affects the LSB flame both through the fluid mechanics of the flow and the kinetics of the chemical reactions in the flame. The effect of the combustor pressure on the fluid mechanics of the LSB flow field can be captured by its effect on the Reynolds number. As noted in Section 3.2, however, previous work indicated the Reynolds number may not be an important parameter for the LSB, particularly in the near field where the flame stabilization occurs. On the other hand, the effect of the combustor pressure on reaction rates in the flame is clearly important. Increasing the combustor pressure results in a lower laminar flame speed and reduced flame thickness for methane-air flames. According to the modified Damköhler model discussed earlier, the reduced laminar flame speed should have little or no effect on the flow field, since the contribution from S_L in Equation FIXME is vanishingly small, even at the lowest reference velocities of our test conditions. However, as suggested by our discussion in Section 3.1, the validity of the simple model at elevated pressure conditions is questionable.

In order to resolve the uncertainties regarding how the LSB flame responds to combustor pressure, the flame was imaged over a range of operating conditions from 3 to 12 atm. For these tests, the reference velocity and the equivalence ratio were held constant. However, the temperature of the reactants continues to increase with pressure. The reason for this was discussed in Chapter FIXME 3 and is attributable to the reduced heat losses in the connecting pipes at the high flow rates required to pressurize the LSB. The flame location and shape inferred from the flame images are presented in Figure FIXME.

At low to moderate pressures, the flame location is nearly invariant for S_{37°, but moves upstream for the S_{45° cases. This behavior can be explained as follows. The flame stabilization location for the S_{45° swirler is closer to the dump plane compared to the S_{37° swirler. This should result in enhanced heat transfer to the dump plane and consequently to the incoming reactants. This feedback is even more effective as the temperature of the incoming reactants increases. This causes the upstream shift of the S_{45° flame, while the S_{37° flame is less affected by these processes.

At high pressures, however, both flames are observed to move downstream, despite the increasing preheat temperatures. The apparent decrease in the turbulent flame speed at these conditions is an unexpected result, and the modified Damköhler model is insufficient in accounting for this observation. Figure FIXME also shows that the flame angle for both cases decreases slightly with pressure. This suggests that the turbulent flame speed was consistently decreasing with pressure. In light of this, the nearly constant location of the S_{37° flame could be attributed to the effects of increasing combustor pressure and preheat temperature nearly canceling each other out at the lower pressures.

3.6 Flame structure

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APPENDIX A

SEEDER DESIGN

A new seeder was designed for use in high pressure implementations of diagnostic techniques like Laser Doppler Velocimetry (LDV), Particle Image Velocimetry (PIV), etc.

The previous design, as shown in Figure FIXME, was a fluidized bed seeding generator. Seeding particles in a cylindrical vessel are fluidized by an air-turbine vibrator. Air is introduced into the vessel in the form of two opposing jets directed tangentially to produce a small amount of swirl in the flow field. Particles are picked up by the air flow and the swirl aids in separating the heavy/coagulated clumps of seeding particles by centrifugal acceleration.

This design had several shortcomings. First, it is observed that the seeding density of the seeded flow generally decreases over time, even if the seeding particles have not been depleted. The seeding particles tend to coagulate over time, due to the buildup of moisture, static charge, etc. In such cases, the vibrator can no longer effectively fluidize the particles. Further, the tangential introduction of the air flow preferentially depletes particles near the walls of the container, leaving the center relatively undisturbed. The cumulative effect of these phenomena diminishes the effectiveness of the seeder.

Second, the fluidized bed requires a minimum amount of seeding particles to function effectively. This requires the seeder to be refilled even before all the seeding particles are consumed.

Third, when designed for high pressure applications, the seeder will become quite heavy due to flanges and other fittings. Such a setup cannot be easily fluidized using a reasonable-sized air-turbine vibrator.

The new seeder design is shown in Figure FIXME, and resembles a funnel with a swirler located halfway up the stem. A perforated base plate holds the swirler and the seeding particles in the conical section of the swirler. Due to the steep angle of the sides of the conical section, the seeding particles continuously collapse into the central section. This negates any need for vibrating the system. Air is introduced from the bottom of the seeder and enters the vessel by passing through the swirler. Since all the air enters this way, there is a considerable amount of swirl in the resulting flow field, Heavy/coagulated seeding particles are flung outward, while lighter particles are carried with the air. After a sufficient distance to allow for the cyclonic separation to be effective, the seeded air passes through another perforated plate which further limits the presence of large clumps of particles. The exiting air is now spatially and temporally uniformly seeded.

APPENDIX B

CH PLIF QUENCHING MODEL

In order to calculate the intensity of the quenched CH PLIF signal in a flame, an improved model of the CH system was constructed and analyzed. According to this new model, CH radicals from the X ground state are excited to the $B(0)$ upper state. This is followed by collisional transfer to the $A(1)$ and $A(0)$ states. The transfer between the nearly degenerate $A(1)$ and $B(0)$ states is partially reversible. The transfer between $B(0)$ and $A(0)$ is not reversible. This is followed by spontaneous emission as CH radicals transition from the A states to the X state. This results in a pseudo-three-level model as shown in Figure FIXME.

Figure FIXME indicates the rates of the various processes discussed. The subscripts 0, 1 and 2 represent the electronic energy levels X, A and B respectively. Processes involving the $A(0)$ state are differentiated from those involving the $A(1)$ state by a prime ('). With the exception of the nearly degenerate $A(1)$ and $B(0)$ states, most collisional excitation steps are neglected due to their low probability.

In this formulation, the signal intensity of the CH PLIF emission is given by Equation B.1.

$$S = (n_1 A_{10} + n_1' A_{10}' + n_2 A_{20})V \tag{B.1}$$

The spontaneous emission coefficients, A_{10}, A_{10}' and A_{20} are obtained from various published papers[8, 9, 10]. The values used for this analysis are presented in Table B.1.

Equations B.2–B.4 describe the time variation of the number density of CH radicals in each excited state.

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Table B.1: *The coefficients of spontaneous emission for transitions in the CH system are provided.*

Transition	Symbol	A, s^{-1}
$B \to X(0,0)$	A_{20}	2.963×10^6
$A \to X(1,1)$	A_{10}	1.676×10^6
$A \to X(0,0)$	A'_{10}	1.832×10^6

$$\frac{dn_1}{dt} = -(A_{10} + Q_{10} + R_{12})n_1 + R_{21}n_2 \tag{B.2}$$

$$\frac{dn'_1}{dt} = -(A'_{10} + Q'_{10})n'_1 + R'_{21}n_2 \tag{B.3}$$

$$\frac{dn_2}{dt} = W_{02}n_0 + R_{12}n_1 - (A_{20} + Q_{20} + R_{21} + R'_{21})n_2 \tag{B.4}$$

At steady state, the rate of change of the number density is minimal. Under this assumption, the LHS of Equations B.2–B.4 can be set to zero. This results in a closed set of linear equations in terms of the populations of the upper states. This set of equations is presented in Equation B.5.

$$\begin{bmatrix} A_{10} + Q_{10} + R_{12} & 0 & -R_{21} \\ 0 & A'_{10} + Q'_{10} & -R'_{21} \\ -R_{12} & 0 & A_{20} + Q_{20} + R_{21} + R'_{21} \end{bmatrix} \begin{bmatrix} n_1 \\ n'_1 \\ n_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ W_{02}n_0 \end{bmatrix} \tag{B.5}$$

The solution to Equation B.5 is shown in Equations B.6–B.8.

$$n_1 = \frac{R_{21}}{(A_{10} + Q_{10} + R_{12})(A_{20} + Q_{20} + R_{21} + R'_{21}) - R_{12}R_{21}} W_{02}n_0 \tag{B.6}$$

$$n'_1 = \frac{(A_{10} + Q_{10} + R_{12})R'_{21}}{(A'_{10} + Q'_{10})((A_{10} + Q_{10} + R_{12})(A_{20} + Q_{20} + R_{21} + R'_{21}) - R_{12}R_{21})} W_{02}n_0$$
$$\tag{B.7}$$

$$n_2 = \frac{(A_{10} + Q_{10} + R_{12})}{(A_{10} + Q_{10} + R_{12})(A_{20} + Q_{20} + R_{21} + R'_{21}) - R_{12}R_{21}} W_{02}n_0 \tag{B.8}$$

These expressions can be further simplified by noting various observations made in studies of the CH system. For instance, previous work[11, 12] has reported that the B state is slightly (about 1.3 times) more prone to quenching compared to the A state. We can thus make the following assumptions.

$$Q_{10} = Q'_{10} = Q \tag{B.9}$$

$$Q_{20} = 1.3Q \tag{B.10}$$

Next, it has been reported[13] that the electronic energy transfer rate from B to A state accounts for 0.24 times the total collisional removal from the B state.

$$\frac{R_{21} + R'_{21} - R_{12}}{Q_{20} + R_{21} + R'_{21} - R_{12}} = 0.24 \tag{B.11}$$

$$\therefore \frac{R_{21} + R'_{21} - R_{12}}{Q} = 0.4105 \tag{B.12}$$

We further know[12, 13] that the collisional transfer from the $B(0)$ energy level populates the nearly degenerate $A(1)$ level about four times faster than the $A(0)$ level.

$$\frac{R_{21} - R_{12}}{R'_{21}} = 4 \tag{B.13}$$

Finally, it was observed[12] that the rate of forward transfer from $B(0)$ to $A(1)$ is about 1.6 times the reverse process.

$$\frac{R_{21}}{R_{12}} = 1.6 \tag{B.14}$$

Collating Equations B.12–B.14, we obtain a closed set of linear equations. This can be solved to eliminate R_{21}, R_{12} and R'_{21} in terms of Q as shown in Equation B.15.

$$\begin{bmatrix} R_{21} \\ R'_{21} \\ R_{12} \end{bmatrix} = \begin{bmatrix} 5.1966 \\ 0.4872 \\ 3.2479 \end{bmatrix} Q \tag{B.15}$$

Substituting Equations B.9, B.10 and B.15 into Equations B.6–B.7 leads to simplified expressions for the populations of the upper electronic states purely as a function of the respective Einstein coefficients and the collisional quenching rate. These are presented in the following Equations B.16–B.18.

$$n_1 = \frac{5.1966Q}{(A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q} W_{02} n_0 \tag{B.16}$$

$$n'_1 = \frac{0.4872Q(A_{10} + 4.2479Q)}{(A'_{10} + Q)\left((A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q\right)} W_{02} n_0 \tag{B.17}$$

$$n_2 = \frac{(A_{10} + 4.2479Q)}{(A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q} W_{02} n_0 \tag{B.18}$$

The quenching rate, Q of excited CH radicals is calculated by using the quenching cross-sections of various species. The quenching cross-sections are measures of the effectiveness of each collision between a given species and an excited CH radical. The effectiveness of the collision also depends on the velocity of collision between the two species, g_j and the abundance of the species, n_j. This relationship is formalized in Equation B.19.

$$Q = \sum_j g_j \sigma_j n_j$$

$$Q = \sum_j \sqrt{\frac{8kT}{\pi \mu_j}} \sigma_j \frac{p N_A}{RT} X_j \qquad \text{(B.19)}$$

In Equation B.19, μ_j represents the reduced mass of the colliding CH-j molecules,p is the pressure, N_A is Avogadro's Number, R is the Universal Gas Constant, T is the temperature, and X_j is the mole fraction of species j. The mole fractions of the various species in the flame, as well as the temperature across the flame are obtained from Chemkin simulations. The expression for the reduced mass is given in Equation B.20.

$$\mu_j = \frac{m_j m_{CH}}{m_j + m_{CH}} \qquad \text{(B.20)}$$

The quenching cross-sections of various species are obtained from various published papers[14, 15, 16] and are functions of temperature. The functional forms used in this study are presented in Table B.2.

The term $W_{02} n_0$ in Equations B.16–B.18 represents the rate of pumping of the ground state CH radicals. The current excitation scheme targets multiple transitions in the R-bandhead. The pumping rate for each transition is the product of the number of CH radicals present in the appropriate level, the Einstein absorption coefficient for that energy level, B_i and the amount of laser energy available at the appropriate frequency, E_i. As a result, the term is actually a summation over the individual energy levels. Equation B.21 presents this symbolically.

Table B.2: *The functional form of the quenching cross-sections of various species with CH are provided.*

Species	σ, Å^2
H_2	$6.1 \exp\left(-686/T\right)$
H	$221 T^{-0.5} \exp\left(-686/T\right)$
O_2	$8.61 \times 10^{-6} T^{1.64} \exp\left(867/T\right)$
OH	$221 T^{-0.5} \exp\left(-686/T\right)$
H_2O	9.6
CH_4	$52.8 T^{-0.5} \exp\left(-84/T\right)$
CO	8.31
CO_2	$8.67 \times 10^{-13} T^{3.8} \exp\left(854/T\right)$
C_2H_6	13.4
N_2	$1.53 \times 10^{-4} T^{1.23} \exp\left(-522.1/T\right)$
C_3H_8	22

$$W_{02}n_0 = \sum_i B_i I_i n_i$$

$$W_{02}n_0 = \sum_i B_i \frac{E_i}{A_c} \frac{pN_A X_{CH}}{RT} f_i \tag{B.21}$$

Table B.3 presents the values of B_i for the transitions targeted by the current excitation scheme.[17] Assuming a Gaussian line shape for the laser, and using the line strengths from LIFBASE, the relative amount of energy absorbed by each transition can be calculated. These values are also presented in Table B.3.

In Equation B.21, A_c is the area of cross-section of the laser beam and f_i is the Boltzmann fraction of the population at the energy level i. The expression for the Boltzmann fraction at the energy level corresponding to the vibrational quantum number v and rotational quantum number J is given in Equation B.22.

$$f(v, J) = \frac{\exp\left(\frac{-hcE_v(v)}{kT}\right)(2J+1)\exp\left(\frac{-hcE_r(v,J)}{kT}\right)}{Q_{rv}} \tag{B.22}$$

Table B.3: *The coefficients of absorption for selected transitions in the CH $X(v = 0)$ system are provided.*

N''	λ, nm	B, m^{2}J^{-1}s^{-1}	E (normalized)
R1			
5	387.2698	7.677×10^9	0.0568
6	387.1899	7.665×10^9	0.1706
7	387.1677	7.610×10^9	0.1483
8	387.206	7.519×10^9	0.1479
9	387.308	7.397×10^9	0.0126
R2			
5	387.2289	7.539×10^9	0.1080
6	387.1549	7.569×10^9	0.1128
7	387.1371	7.539×10^9	0.0841
8	387.1786	7.464×10^9	0.1311
9	387.283	7.354×10^9	0.0279

The vibrational energy, $E_v(v)$ of a level is calculated according to Equation B.23, while the rotational energy, $E_r(v, J)$ is calculated according to Equation B.24.

$$E_v(v) = \omega_e \left(v + \frac{1}{2}\right) - \omega_e x_e \left(v + \frac{1}{2}\right)^2 + \omega_e y_e \left(v + \frac{1}{2}\right)^3 - \omega_e z_e \left(v + \frac{1}{2}\right)^4 \quad \text{(B.23)}$$

$$E_r(v, J) = \left\{ B_e - \alpha_e \left(v + \frac{1}{2}\right) \right\} J(J+1) - \left\{ D_e + \beta_e \left(v + \frac{1}{2}\right) \right\} J^2(J+1)^2 \quad \text{(B.24)}$$

The spectroscopic constants in Equations B.23 and B.24 are found in literature[18] and are provided here in Table B.4.

The rovibrational partition function, Q_{rv} is a summation over all available vibrational and rotational levels in the particular electronic state. For the ground state of the CH molecule, there are five available vibrational quantum numbers, $v = 0$ to $v = 4$. The CH system falls under Hund's Case b and hence, the appropriate rotational quantum number to use is N. Each vibrational level has twenty-two possible values for N from $N = 1$ to $N = 22$. For each rotational quantum number N, there are two possible values of J given by $N \pm \frac{1}{2}$.

Table B.4: *Spectroscopic constants for the CH $X^2\Pi$ level are presented.*

Constant	Value, cm^{-1}
ω_e	2860.7508
$\omega_e x_e$	64.4387
$\omega_e y_e$	0.36345
$\omega_e z_e$	-1.5378×10^{-2}
B_e	14.459883
α_e	0.536541
D_e	1.47436×10^{-3}
β_e	-2.530×10^{-5}

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