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

A Dissertation Presented to The Academic Faculty

by

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LIST OF SYMBOLS

 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 1.1.

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 | | | |
|-----------------------------------|--------------------|--------------------|--|--|
| | $S_{37^{\circ}}$ | $S_{45^{\circ}}$ | | |
| Swirler data | | | | |
| Outer diameter, d_s , mm | 38 | 38 | | |
| Diameter ratio, $\frac{d_i}{d_c}$ | 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.

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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.

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

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The details of Configuration B are shown in Figure FIXME.

1.2 High Pressure Test Rig

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

1.2.1 Test Rig A 51

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

The combustor pressure and temperature are measured at the head of the inlet nozzle by a pressure transducer and a thermocouple respectively. In addition, the upstream pressure and the pressure differential are measured at the air and fuel orifice flow meters. For the preheated air stream, the upstream temperature is also measured. The measurements are used to calculate the four primary flow parameters (combustor pressure, preheat temperature, reference velocity and equivalence ratio) for the LSB in real time. All measurements are monitored and recorded during the course of the experiment by a LabView VI.

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

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

1.2.2 Test Rig B

A schematic of Test Rig B is shown in Figure FIXME. Both test rigs share the same upstream supply of preheated air, cold air and natural gas. The preheated air splits into two separate streams a short distance after mixing with the natural gas fuel. Orifice flow meters are used to meter the fuel flow and each individual reactant stream. Each orifice flow meter is equipped with a thermocouple, an upstream pressure transducer and a differential pressure transducer. The cooling air for the co-flow is not

metered. All measurements are monitored and recorded by a LabView VI.

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

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

1.3 Diagnostics

1.3.1 Laser Doppler Velocimetry

The velocity field of the LSB is mapped using a TSI 3-component LDV system. Three wavelengths (514 nm, 488 nm and 476 nm) are separated from the output of a 5 W Argon ion laser by an FBL-3 multicolor beam generator. The individual beams are split into two coherent beams which are then focused to intersect and produce interference fringes within an ellipsoidal measurement volume with dimensions of the order of 100 μ m. For this purpose, two transceiver probes are mounted 90° apart about the axis of the LSB. One transceiver probe focuses the 514 nm and 488 nm beams in planes perpendicular to each other, while the second probe focuses the 476 nm beams orthogonal to the other two beams. Particles in the flow field crossing the interference fringes scatter the laser light elastically and produce a sinusoidal signal whose frequency is proportional to the velocity of the particle. The transceiver probes collect this scattered light and each wavelength is detected separately by a PDM-

1000-3 three-channel photodetector module. The output from the photodetector is processed by an FSA-3500-3 signal processor. The resulting three components of the particle/flow velocity are recorded by the FlowSizer software.

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Since the airflow is very sparsely populated by particles, the flow needs to be artificially seeded to facilitate LDV measurements in a reasonable amount of time. The seeding particles to be used and their mean diameter are decided by the characteristics of the flow to be imaged. [2] Since the LSB flow field is a reacting one, the particles need to have high melting points. Further, the particles need to be small enough to follow the flow closely and large enough or reflective enough to scatter light efficiently in the measurement volume. Based on these requirements, commercially available alumina particles with a mean particle diameter of 5 μ m were chosen for this study. In order to uniformly seed the flow, a novel seeding generator was designed as described in Appendix A. The seeding particles were introduced slightly upstream of 126 the 1.8 m (6 ft) long straight pipe section in Test Rig A.

LDV data is only acquired at atmospheric pressure conditions. At high pressure conditions, the reacting LSB flow field produces sharp refractive index gradients that rapidly shift in the turbulent flow field. This causes strong beam steering effects making it very difficult for the laser beams to reliably intersect within such a small measurement volume. The long distance traveled by the beams in the test rig further exacerbated this problem, making LDV data nearly impossible to acquire at such conditions.

1.3.2 CH* chemiluminescence

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

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

1.3.2.1 Image Processing

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

Even when background-corrected, the walls of the combustor are not at zero intensity in the average chemiluminescence image. This is particularly noticeable near the dump plane where there is no flame present and yet the walls are clearly illuminated. The source of this illumination is mostly scattered chemiluminescence from the flame itself, and to a lesser degree, blackbody radiation from the heated walls. The

averaged chemiluminescence image allows us to measure the flame standoff distance by following the intensity profile along the centerline of the combustor. The intensity profile rises sharply when passing the flame standoff location. Thus, the flame standoff location can be ascertained by finding the inflection point in the intensity profile.

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

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

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

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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 Actor 512×512 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 micrometer was found to be inaccurate. This required the recalibration of the laser in order to know the slope and offset of the calibration curve.

An Ocean Optics HR 2000 spectrometer is used to get the true wavelength of the laser output. The spectrometer is pre-calibrated using 50 wavelengths in the 400–850 nm range from output of an Neon discharge lamp source. The spectrometer is also

intensity corrected over this range using a black body source. The estimated error in the resolution of the device is about 0.1 nm (1 Å).

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

1.3.3.2 Excitation scan

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

In order to do this, the CH PLIF imaging system, consisting of the alexandrite laser and the intensified PI Acton 512×512 camera is used to image a premixed, stoichiometric, laminar methane-air flame. The laminar flame is stabilized on a Bunsen burner with an inner diameter of 10.16 mm (0.4 in). The alexandrite laser is operated at 10 Hz, with a power of 16 mJ/pulse. The second harmonic beam is refracted into a sheet about 25 mm tall, with a thickness on the order of 100 μ m passing through the center of the flame. The edges of the sheet are blocked by razor blades.

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

is approximately 62 μ m per pixel.

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

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

1.3.3.3 Linearity test

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

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

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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 — $A o X(1,1), \ A o X(0,0)$ and B o 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 309 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.

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- 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 ac-329 count 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 332 measured in experiments done so far.

¹In 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

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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 $_{344}$ equivalence ratio of the premixed reactants, ϕ . We further introduced a geometric 345 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 357 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.

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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 $S_{37^{\circ}}$ swirler was used. In a parallel series of tests, the $S_{45^{\circ}}$ 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, $S_{37^{\circ}}$ 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 $S_{45^{\circ}}$ 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 Figure FIXME. While increasing the reference velocity did not affect the turbulent combustion regime at lower pressures in a flamelet combustion regime, at elevated pressures the flame may be transitioning into the thin reaction zone regime. This transition would cause a reduction in S_T/S_L , or at least a lesser increase, and the turbulent flame speed would no longer be expected to increase in step with U_0 and the increased levels of turbulence. This would explain the the observed downstream shift of the high pressure LSB flame at high reference velocities.

3.2 Effect of preheat temperature

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

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

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

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

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

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

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

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 $S_{45^{\circ}}$ 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 $S_{37^{\circ}}$ swirler.

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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 $S_{45^{\circ}}$ swirler stabilizes a flame closer to the dump plane and with a larger flame angle compared to the $S_{37^{\circ}}$ swirler.

This result highlights an interesting trade-off for the designers of LSB-based gas turbine engines. The $S_{45^{\circ}}$ flame is located further upstream and has a more concentrated 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 $S_{45^{\circ}}$ flame is more stable and will resist perturbations in the incoming flow better than the $S_{37^{\circ}}$ flame. However, the presence of a strong recirculation zone in the flow field of the $S_{45^{\circ}}$ 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 $\mathrm{NO_{x}}$ performance of the $S_{45^{\circ}}$ swirler will be degraded compared to the $S_{37^{\circ}}$ swirler. The trade-off for gas turbine 461

engine designers is thus between flame stability and emissions performance.

3.4 Effect of equivalence ratio

The LSB is primarily intended for fuel-lean operation in order to utilize its low NO_x 464 emission performance. As a result, most of the testing was done as close as possible to a target ϕ of 0.56. Limited testing was carried out at 12 atm for two off-target conditions: a slightly richer ($\phi \approx 0.58$) and a slightly leaner ($\phi \approx 0.53$) mixture, in 467 order to explore the sensitivity of the LSB flame to limited changes in equivalence ratio. The $S_{45^{\circ}}$ swirler was used for these tests. The corresponding averaged and Abel-deconvoluted flame images are presented in Figure FIXME.

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

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

It should be noted that the reliance on a toroidal recirculation zone to anchor the flame to the inlet is one of the primary flame stabilization mechanisms used by 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 $S_{37^{\circ}}$, but moves upstream for the $S_{45^{\circ}}$ cases. This behavior can be explained as follows. The flame stabilization location for the $S_{45^{\circ}}$ swirler is closer to the dump plane compared to the $S_{37^{\circ}}$ 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 $S_{45^{\circ}}$ flame, while the $S_{37^{\circ}}$ 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 $S_{37^{\circ}}$ 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

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.

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

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

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

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

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

$$\frac{dn_2}{dt} = W_{02}n_0 + R_{12}n_1 - (A_{20} + Q_{20} + R_{21} + R'_{21})n_2$$
(B.2)
$$\frac{dn_2}{dt} = W_{02}n_0 + R_{12}n_1 - (A_{20} + Q_{20} + R_{21} + R'_{21})n_2$$
(B.3)

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

At steady state, the rate of change of the number density is minimal. Under this 590 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. 593

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

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

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

$$n_{1}' = \frac{(A_{10} + Q_{10} + R_{12})R_{21}'}{(A_{10}' + Q_{10}')((A_{10} + Q_{10} + R_{12})(A_{20} + Q_{20} + R_{21} + R_{21}') - R_{12}R_{21})}W_{02}n_{0}$$
(B.7)

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

These expressions can be further simplified by noting various observations made 595 in studies of the CH system. For instance, previous work[11, 12] has reported that 596 the B state is slightly (about 1.3 times) more prone to quenching compared to the A 597 state. We can thus make the following assumptions.

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

$$Q_{20} = 1.3Q (B.10)$$

Next, it has been reported[13] that the electronic energy transfer rate from B to $_{599}$ A state accounts for 0.24 times the total collisional removal from the B state.

$$\frac{R_{21} + R'_{21} - R_{12}}{Q_{20} + R_{21} + R'_{21} - R_{12}} = 0.24$$
(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 for populates the nearly degenerate A(1) level about four times faster than the A(0) level.

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

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. 604

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

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.

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

Substituting Equations B.9, B.10 and B.15 into Equations B.6–B.7 leads to simplifield expressions for the populations of the upper electronic states purely as a function 608 of the respective Einstein coefficients and the collisional quenching rate. These are 609 presented in the following Equations B.16–B.18. 610

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

$$n_{1} = \frac{5.1966Q}{(A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q} W_{02}n_{0}$$

$$n'_{1} = \frac{0.4872Q(A_{10} + 4.2479Q)}{(A'_{10} + Q)((A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q)} W_{02}n_{0}$$

$$n_{2} = \frac{(A_{10} + 4.2479Q)}{(A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q} W_{02}n_{0}$$
(B.16)
$$n_{3} = \frac{(A_{10} + 4.2479Q)}{(A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q} W_{02}n_{0}$$
(B.17)

$$n_2 = \frac{(A_{10} + 4.2479Q)}{(A_{10} + 4.2479Q)(A_{20} + 6.9838Q) - 16.8780Q} W_{02} n_0$$
(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 612 effectiveness of each collision between a given species and an excited CH radical. The 613 effectiveness of the collision also depends on the velocity of collision between the two 614 species, g_j and the abundance of the species, n_j . This relationship is formalized in 615 Equation B.19. 616

$$Q = \sum_{j} g_{j} \sigma_{j} n_{j}$$

$$Q = \sum_{j} \sqrt{\frac{8kT}{\pi \mu_{j}}} \sigma_{j} \frac{pN_{A}}{RT} X_{j}$$
(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.

$$\mu_j = \frac{m_j m_{CH}}{m_j + m_{CH}} \tag{B.20}$$

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 | $\sigma, \mathring{ m A}^2$ |
|------------------------------|---|
| $\overline{\mathrm{H}_{2}}$ | $6.1 \exp(-686/T)$ |
| Н | $221T^{-0.5}\exp\left(-686/T\right)$ |
| O_2 | $8.61 \times 10^{-6} T^{1.64} \exp{(867/T)}$ |
| OH | $221T^{-0.5}\exp\left(-686/T\right)$ |
| H_2O | 9.6 |
| $\overline{\mathrm{CH}_{4}}$ | $52.8T^{-0.5}\exp\left(-84/T\right)$ |
| CO | 8.31 |
| CO_2 | $8.67 \times 10^{-13} T^{3.8} \exp(854/T)$ |
| $C_2 \bar{H_6}$ | 13.4 |
| N_2 | $1.53 \times 10^{-4} T^{1.23} \exp(-522.1/T)$ |
| C_3H_8 | 22 |

$$W_{02}n_{0} = \sum_{i} B_{i}I_{i}n_{i}$$

$$W_{02}n_{0} = \sum_{i} B_{i}\frac{E_{i}}{A_{c}}\frac{pN_{A}X_{CH}}{RT}f_{i}$$
(B.21)

Table B.3 presents the values of B_i for the transitions targeted by the current 633 excitation scheme. [17] Assuming a Gaussian line shape for the laser, and using the line 634 strengths from LIFBASE, the relative amount of energy absorbed by each transition 635 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 637 Boltzmann fraction of the population at the energy level i. The expression for the 638 Boltzmann fraction at the energy level corresponding to the vibrational quantum 639 number v and rotational quantum number J is given in Equation B.22.

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

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

| N'' | λ , nm | $B, \mathrm{m^2 J^{-1} s^{-1}}$ | 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, 641 while the rotational energy, $E_r(v, J)$ is calculated according to Equation B.24. 642

$$E_{v}(v) = \omega_{e} \left(v + \frac{1}{2}\right) - \omega_{e} x_{e} \left(v + \frac{1}{2}\right)^{2} + \omega_{e} y_{e} \left(v + \frac{1}{2}\right)^{3} - \omega_{e} z_{e} \left(v + \frac{1}{2}\right)^{4}$$
 (B.23)

$$E_{r}(v, J) = \left\{B_{e} - \alpha_{e} \left(v + \frac{1}{2}\right)\right\} J(J+1) - \left\{D_{e} + \beta_{e} \left(v + \frac{1}{2}\right)\right\} J^{2} (J+1)^{2}$$
 (B.24)

The spectroscopic constants in Equations B.23 and B.24 are found in literature [18] 643 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 |
| $lpha_e$ | 0.536541 |
| D_e | 1.47436×10^{-3} |
| eta_{e} | -2.530×10^{-5} |

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