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

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CHAPTER 1

CH PLIF SIGNAL MODELING AND VALIDATION

1.1 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 — $A \rightarrow X(1,1)$, $A \rightarrow X(0,0)$ and $B \rightarrow X(0,1)$. 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 A.1.

$$S = nVA \tag{1.1}$$

In Equation A.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 2

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 is imaged over a range of operating conditions and the effect of flow and geometric parameters on the reacting flow field is investigated. This results of the investigation are presented in this chapter.

2.1 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 earlier

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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 standoff distance. This result is very desirable for gas turbine designers, since the flame location and shape can be assumed to be constant. Limited testing conducted in earlier works confirms 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. The increase in reference velocity continues to produces 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.

However, when the $S_{45°}$ swirler was tested at higher reference velocities, 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.

To examine the probable cause of this limitation more closely, consider the effect of increasing the reference velocity on the turbulent combustion regime where 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

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in Figure FIXME. While previously, increasing the reference velocity did not affect the turbulent combustion regime, at elevated pressures, the flame is more likely to transition into the thin reaction zone. This transition causes a drop-off in the S_T/S_L plot and the turbulent flame speed no longer increases in step with the increased levels of turbulence. This results in the observed downstream shift of the high pressure LSB flame at high reference velocities.

2.2 Effect of preheat temperature

The preheat temperature of the reactants is a key flow parameter for the LSB due to two reasons. First, The temperature of the incoming flow directly affects its viscosity and consequently, the velocity field. Additionally, the rates of most chemical reactions in the flame zone are acutely sensitive to the temperature of the reactants. 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 successive runs.

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[1] 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.

These results suggest that holding S_T constant, 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 reality, 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 or otherwise, 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.

2.3 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 147 smaller holes. The net effect retains the same mass flow split as in the $S_{37°}$ swirler. 148

Earlier, in Chapter FIXME 2, we discussed how the swirler vane angle relates to 149 the amount of swirl imparted to the incoming flow. According to Equation FIXME, a 150 swirler with a higher vane angle will produce greater swirl in the reactants. Previous 151 work in swirl combustion[2, 3] has pointed out that increased swirl shortens the flame 152 by enhancing the swirl-induced radial pressure gradients. The data acquired in the 153 present investigation is in agreement with this observation. Operated at identical 154 inlet conditions, the $S_{45°}$ swirler stabilizes a flame closer to the dump plane and with 155 a larger flame angle compared to the $S_{37°}$ swirler. 156

This result highlights an interesting trade-off for the designers of LSB-based gas 157 turbine engines. The $S_{45°}$ flame is located further upstream and has a more concen- 158 trated region of heat release. This enhances the strength of the toroidal recirculation 159 zone near the dump plane, which may be powerful enough under certain conditions 160 (as we shall see in the Section 2.4) to even cause the flame to attach itself to the 161 lip of the inlet. All of this means that the $S_{45°}$ flame is more stable and will resist 162 perturbations in the incoming flow better than the $S_{37°}$ flame. However, the presence 163 of a strong recirculation zone in the flow field of the $S_{45°}$ swirler will entrain more hot 164 products and retain them longer near the zone of heat release. This is a recipe for 165 the production of thermal NO_x. While no emission measurements were made as part 166 of this study, it may be reasonably anticipated that the NO_x performance of the $S_{45°}$ 167 swirler is worse than the $S_{37°}$ swirler. The trade-off for gas turbine engine designers 168 is thus between flame stability and emissions performance. 169

2.4 Effect of equivalence ratio 170

The LSB is primarily intended for fuel-lean operation in order to utilize its low NO_x 171 emission performance. As a result, most of the testing was done as close to the target 172

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ϕ of 0.56 as possible. However, limited testing was done at 12 atm at both a slightly rich ($\phi \approx 0.58$) and a slightly lean ($\phi \approx 0.53$) condition to explore the sensitivity of the lSB flame to limited changes in equivalence ratio. The $S_{45°}$ swirler was used for these tests. The corresponding averaged and Abel-deconvoluted flame images are presented in Figure FIXME.

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 2.3 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.

2.5 Effect of combustor pressure

In a typical gas turbine application, the combustor pressure is expected to vary 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 of the flow. However, as noted in Section 2.2, 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 the reactions occurring in the flame are more dominant. 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 2.1, 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 atm 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

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moves upstream for the $S_{45°}$ cases. This observation is explained as follows. The ²²³
flame stabilization location for the $S_{45°}$ swirler is closer to the dump plane compared ²²⁴
to the $S_{37°}$ swirler. This results in enhanced heat transfer to the dump plane and ²²⁵
consequently to the incoming reactants. This feedback is even more effective as the ²²⁶
temperature of the incoming reactants increases. This causes the upstream shift of ²²⁷
the $S_{45°}$ flame, while the $S_{37°}$ flame is less affected by these processes. ²²⁸

At high pressures, however, both flames are observed to move downstream, despite ²²⁹
the increasing preheat temperatures. The apparent decrease in the turbulent flame ²³⁰
speed at these conditions is an unexpected result and the modified Damköhler model ²³¹
is insufficient in accounting for this observation. Figure FIXME also shows that the ²³²
flame angle for both cases decreases slightly with pressure. This suggests that the ²³³
turbulent flame speed was consistently decreasing with pressure. In light of this, ²³⁴
the nearly constant location of the $S_{37°}$ flame could be attributed to the effects of ²³⁵
increasing combustor pressure and preheat temperature nearly canceling each other ²³⁶
out at the lower pressures. ²³⁷

2.6 Flame structure ²³⁸

APPENDIX A

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 A.1.

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

The spontaneous emission coefficients, A_{10}, A_{10}' and A_{20} are obtained from various published papers[4, 5, 6]. The values used for this analysis are presented in Table A.1.

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

Table A.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

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

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

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

At steady state, the rate of change of the number density is minimal. Under this assumption, the LHS of Equations A.2–A.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 A.5.

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

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

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

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

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

These expressions can be further simplified by noting various observations made in studies of the CH system. For instance, previous work[7, 8] 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.

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

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

Next, it has been reported[9] that the electronic energy transfer rate from B to A state accounts for 0.24 times the total collisional removal from the B state.

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

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

We further know[8, 9] 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.

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

Finally, it was observed[8] that the rate of forward transfer from $B(0)$ to $A(1)$ is about 1.6 times the reverse process.

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

Collating Equations A.12–A.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 A.15.

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

Substituting Equations A.9, A.10 and A.15 into Equations A.6–A.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 A.16–A.18.

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

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

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

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

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effectiveness of the collision also depends on the velocity of collision between the two 286
species, g_j and the abundance of the species, n_j. This relationship is formalized in 287
Equation A.19. 288

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

$$Q = \sum_j \sqrt{\frac{8kT}{\pi \mu_j}} \sigma_j \frac{pN_A}{RT} X_j \qquad (A.19)$$

In Equation A.19, μ_j represents the reduced mass of the colliding CH-j molecules,p 289
is the pressure, N_A is Avogadro's Number, R is the Universal Gas Constant, T is the 290
temperature, and X_j is the mole fraction of species j. The mole fractions of the 291
various species in the flame, as well as the temperature across the flame are obtained 292
from Chemkin simulations. The expression for the reduced mass is given in Equation 293
A.20. 294

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

The quenching cross-sections of various species are obtained from various pub- 295
lished papers[10, 11, 12] and are functions of temperature. The functional forms used 296
in this study are presented in Table A.2. 297

The term $W_{02}n_0$ in Equations A.16–A.18 represents the rate of pumping of the 298
ground state CH radicals. The current excitation scheme targets multiple transitions 299
in the R-bandhead. The pumping rate for each transition is the product of the number 300
of CH radicals present in the appropriate level, the Einstein absorption coefficient for 301
that energy level, B_i and the amount of laser energy available at the appropriate 302
frequency, E_i. As a result, the term is actually a summation over the individual 303
energy levels. Equation A.21 presents this symbolically. 304

Table A.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

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

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

Table A.3 presents the values of B_i for the transitions targeted by the current excitation scheme.[13] 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 A.3.

In Equation A.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 A.22.

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

Table A.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 A.23, while the rotational energy, $E_r(v, J)$ is calculated according to Equation A.24.

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

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

The spectroscopic constants in Equations A.23 and A.24 are found in literature[14] and are provided here in Table A.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 A.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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