

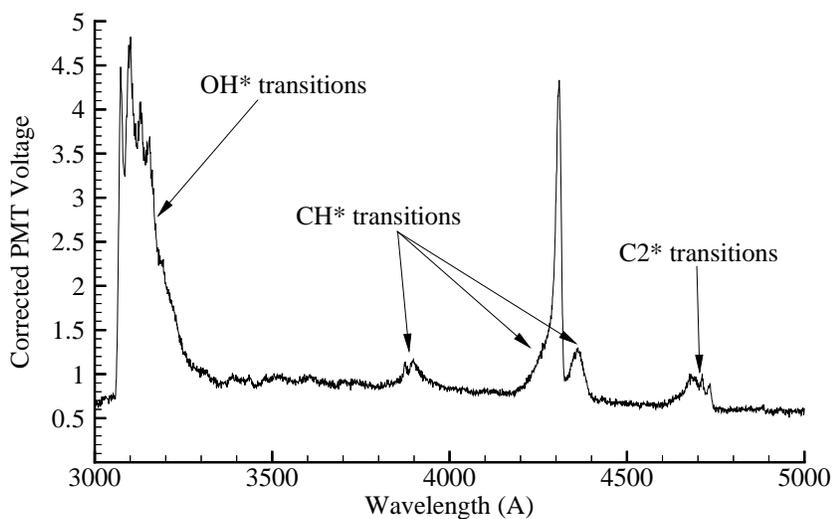
## Chapter 4

# Data Processing and Interpretation

## 4.1 Spectral Content Light Scans

The visible and near ultra-violet light spectrum of a Bunsen burner flame is shown in Figure 4.1. The voltage shown in Figure 4.1 is corrected for the efficiency of the optical system at the different wavelengths. The wavelength dependent transmission losses are discussed in detail in Section 4.2.1. The spectrum was taken at an equivalence ratio of 1.0 and an air-flow rate of 60 cc/sec. The figure shows peaks from the three major diatomic chemiluminescence emitters. OH\* shows the most energy, in three peaks that are closely spaced in the 308 nm range. The three peaks correspond to three so called band-heads. Two CH\* peaks are seen near 380 nm and 431 nm, respectively. The small peak seen just beyond the CH\* peak at 431 nm is due to the accumulation of secondary band heads at this wavelength. (Gaydon, 1974) Only one C<sub>2</sub>\* band-head at 471 nm can be seen. The major C<sub>2</sub>\* band-head at 516.5 nm is not captured because the wavelength range for this particular scan was from 300 nm to 500 nm. C<sub>2</sub>\* is not of great interest in the present study because its formation mechanism is still poorly understood and because C<sub>2</sub>\* emission essentially disappears at lean equivalence ratios. Since the study focuses on developing applications for chemiluminescence measurements in ultra lean premixed (ULPM) type gas turbine combustors, the measurement of C<sub>2</sub>\* is not worthwhile.

Note also the pedestal on top of which the chemiluminescence peaks of OH\* and CH\* sit. The pedestal is due to the chemiluminescence of the more complex molecule of CO<sub>2</sub>\*. The shape of the pedestal is predictable to within 2% given one appropriate voltage measurement. (Clark, 1958) The pedestal is problematic in the present study, because some of the signal measured at 431 nm is due to CO<sub>2</sub>\* chemiluminescence and not due solely to CH\* chemiluminescence. Section 4.2.2 discusses the problem in greater detail. To make the measurement of chemiluminescence practical, complete wavelength scans must be avoided. To determine the relative quantity of transitions for the different chemiluminescence species, all of the energy due to that particular species must be integrated. The integration will reveal for example that OH\* is a much stronger emitter than CH\* for premixed methane flames even though their peak



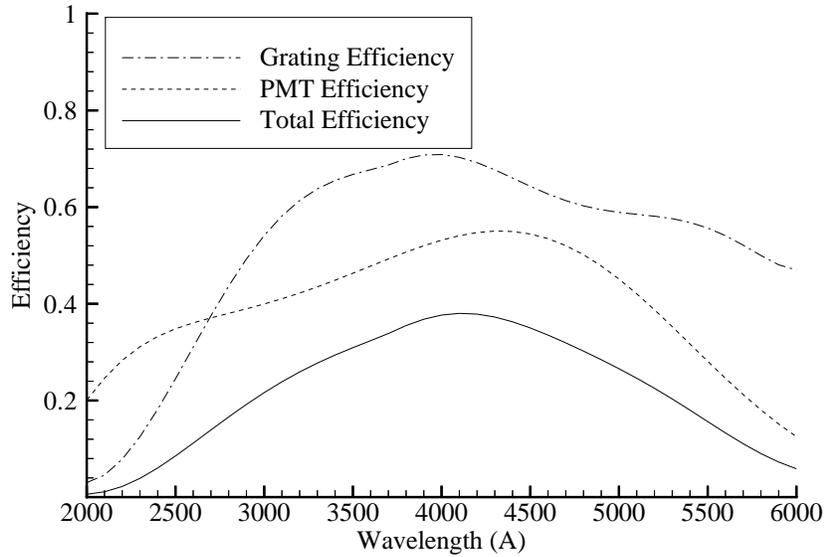
**Figure 4.1:** Chemiluminescence spectrum for a Bunsen burner flame

voltages may be the same. The difference is due to the fact that the area under the OH\* peaks is significantly larger than the area under the CH\* peaks. In order to show that chemiluminescence measurement is a viable option for monitoring in a dynamic environment, the voltage measured at one location in the wavelength spectrum must be shown to be representative of the total energy over all the wavelengths for that species. Section 4.2.2 addresses the issue of integration in much greater detail.

## 4.2 Calibration of Light Signal

### 4.2.1 Light transmission losses

In order to reconstruct a measure of the true chemiluminescence intensity from the measured voltage, all major, wavelength dependent light losses must be accounted for. All three optical components are discussed with respect to these losses in the following paragraphs. The losses are summarized in Figure 4.2. The figure shows individual component losses and a combined system efficiency curve.



**Figure 4.2:** Optical system efficiency

## Monochrometer

The monochrometer grating is more efficient at some wavelengths than others. The efficiency of the monochrometer at different wavelengths is determined by grating characteristics. Gratings are blocks of reflective material that contain grooves. The grooves are cut into the material at an angle which is called the blaze angle. The spacing of the grooves determines the wavelength resolution of the grating. The grating in the Jarrell-Ash monochrometer has 1180 grooves per mm and was blazed for 400 nm. The peak efficiency of the monochrometer is thus near 400 nm, with the efficiency decreasing to either end of the spectrum as shown in Figure 4.2. The resolution given by the grating varies with slit width but can be as fine as 0.05 nm.

## Photomultiplier-tube

The photocathode material of the PMT determines the quantum efficiency of the PMT. The quantum efficiency is a measure of the probability that an incoming photon or particle of light at a certain wavelength will cause the emission of an electron. The

material used in the Hamamatsu R958 PMT was designed for wavelengths from the UV to the near IR (infra-red) wavelength regions. The variation of quantum efficiency with wavelength is shown in Figure 4.2.

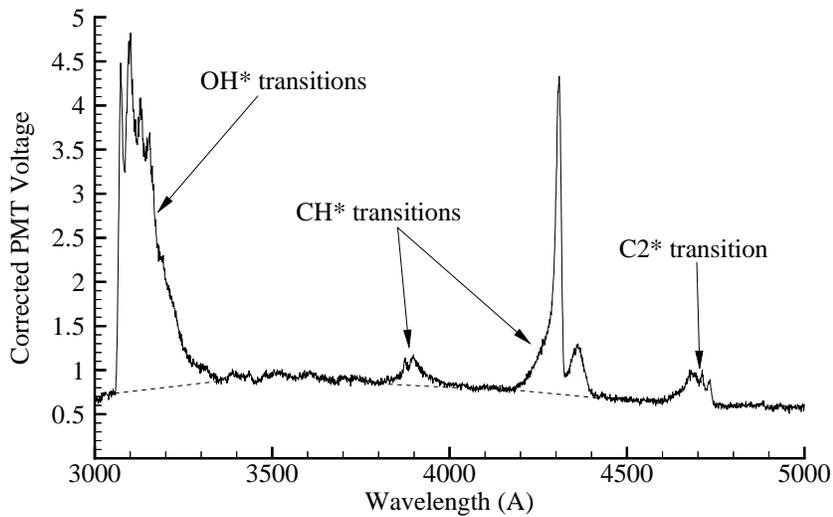
### **Lenses and fiber-optics**

The losses in the remaining optical components such as lenses and fiber-optics do not vary significantly in the wavelength range studied. Lenses and fiber-optic cable are all made of fused-silica to ensure high transmission (greater than 98%) to below 300 nm.

#### **4.2.2 Integration of OH\* and CH\* energy**

As alluded to briefly earlier in Section 4.1, a useful measurement of chemiluminescence must not require a wavelength scan. The relationship between a measured voltage and the total integrated intensity for a certain chemiluminescence species can be determined by experimentation. Using several sets of spectral scans at different conditions and using both the honeycomb burner and the Bunsen burner, the relationship can be examined in detail.

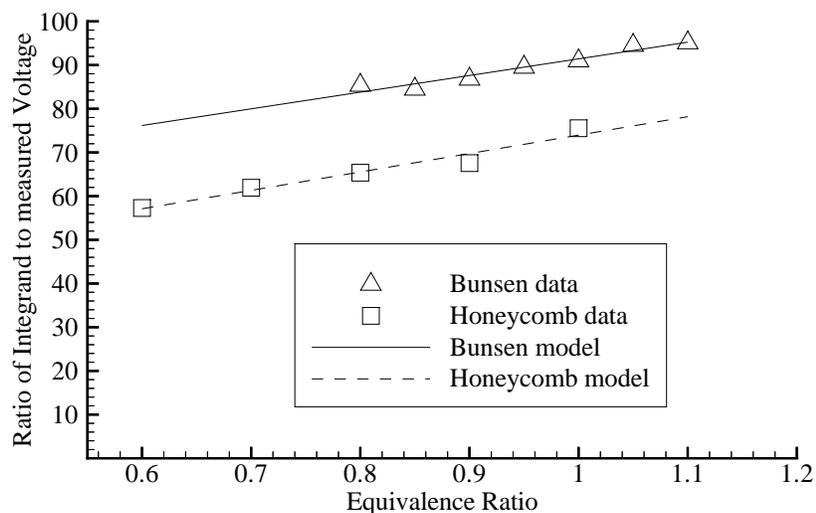
For OH\*, the representative voltage measurement is taken at a wavelength of 308 nm. For CH\*, the representative voltage measurement is taken at a wavelength of 431 nm. The total integrated intensity is then calculated by integrating under the wavelength curve from an appropriate starting wavelength to an appropriate ending wavelength, subtracting an estimate for the background CO<sub>2</sub>\* radiation at every data point. The process is illustrated in Figure 4.3 using the spectrum shown also above in Figure 4.1. The peaks of OH\* and CH\* sit on top of the continuous CO<sub>2</sub>\* chemiluminescence. Under the respective peaks, the chemiluminescence due to CO<sub>2</sub>\* is estimated to be linear (see Figure 4.3). The starting and ending wavelengths are chosen so that the amount of linearly modeled CO<sub>2</sub>\* chemiluminescence and the amount of OH\* and CH\* chemiluminescence not accounted for are both minimized. The result of the integration is a value of V-nm that represents the total amount of energy due to a



**Figure 4.3:** Chemiluminescence spectrum for a Bunsen burner flame with  $\text{CO}_2^*$  continuum estimate

certain molecule's radiative transition. The integration is repeated for several experimental conditions and for both the honeycomb and Bunsen burners. For each integration a ratio may be taken of the integrand value to the measured representative voltage, hereafter referred to as the integrand scale factor. The variation of the integrand scale factor across experimental conditions is a measure of the spectrum shape variation. If the spectrum shape stayed the same always and scaled with the representative voltage then the calculated integrand scale factor would remain the same. Variations in the integrand scale factor thus indicate a change in the spectral shape of the chemiluminescence radiation.

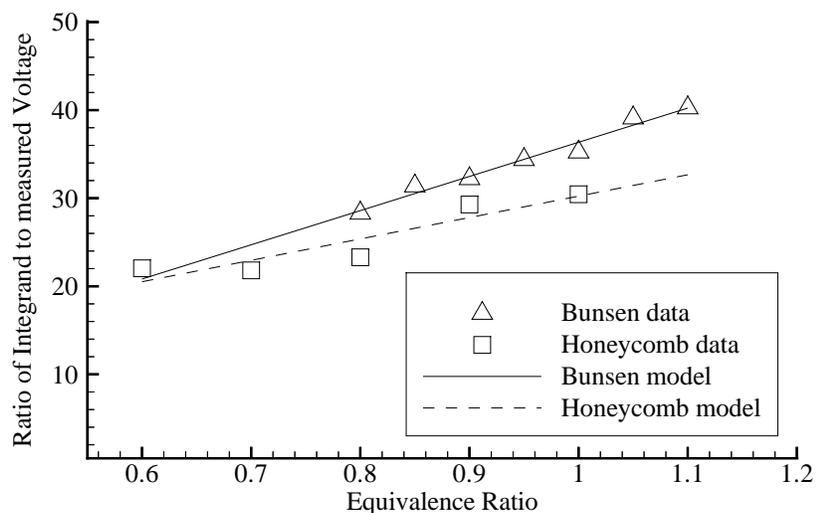
Variations of the integrand scale factor with flow-rate were insignificant. For equivalence ratio variations, there are trends for both  $\text{OH}^*$  and  $\text{CH}^*$ . Figure 4.4 shows the variation of the  $\text{OH}^*$  chemiluminescence integrand scale factor with equivalence ratio for the honeycomb and Bunsen burners. Along with the collected data points, a linear fit for each burner is given. The linear fit in both cases has a  $R^2$  value greater than 0.95, which indicates a high-reliability fit. The slopes of the lines are nearly equal, which indicates that the variation of the integrand scale factor with



**Figure 4.4:** OH\*integrant scale factor variation with equivalence ratio

equivalence ratio is very similar for both burners. The lower offset for the honeycomb burner compared to the Bunsen burner can be explained by examining the flame type in each case. The flow-rates in honeycomb burner dictate that the flame speed for the honeycomb burner be less than 10% of the adiabatic value. The Bunsen burner flame speed varies radially, but averages slightly below the adiabatic flame speed. The flame speed in the honeycomb burner is lowered through very high heat-loss to the burner. The heat-loss to the burner affects the flame speed by lowering the peak temperature in the flame. All reaction rates are lowered by the increased heat-loss, including the reactions producing chemiluminescence, causing the chemiluminescence output on a per unit mass of fuel burned basis from the honeycomb burner to be much lower than that from the Bunsen burner.

The variation of the CH\* chemiluminescence integrant scale factor is shown in Figure 4.5. Along with the collected data points, a linear fit for each burner is given. The linear fit in both cases has a  $R^2$  value greater than 0.85, which indicates a reliable fit. Compared to Figure 4.4, the integrant scale factor for CH\* seems more



**Figure 4.5:** CH\* integrand scale factor variation with equivalence ratio

sensitive to variations in equivalence ratio. The honeycomb burner integrand scale factor again lies below that of the Bunsen burner. In order to explain the difference in slope between the honeycomb burner and the Bunsen burner, the temperature variation with equivalence ratio for the two burners must be considered. The flame speed and therefore the temperature of the Bunsen burner flame varies significantly as the equivalence ratio of the mixture is changed. For the honeycomb burner, the temperature remains fairly steady, since the flame speed does not change appreciably as the equivalence ratio of the mixture is varied. The reason why the difference in slope is more or less absent in the case of OH\*, is that the formation path for OH\* is much less temperature sensitive than the formation path for CH\*, as will be discussed in great in detail in Section 9.1 and Section 9.2.

### 4.2.3 Single wavelength measurement interpretation

The work described in the previous section shows that a voltage measurement taken at an appropriate wavelength can represent the total energy of a chemilumi-

nescent species. The integrand scale factor is a measurable function of equivalence ratio. Single wavelength voltage measurements can now be directly related to the total chemiluminescence energy of the spectrum using the calculated integrand scale factors. The units of the scaled voltage measurement are V-nm.

The final conversion factor from V-nm to total luminous intensity or total chemiluminescence quantum yield is only a function of the burner and the optical system. The conversion factor has to account for the percentage of light lost and not collected (constant for all conditions for the same burner) and the number relating the PMT current to luminous intensity, assuming a 100% quantum efficiency of the PMT. PMT inefficiency has already been accounted for in the voltage correction, see Section 4.2.1.

## 4.3 Chemiluminescence Measurement Correction

### 4.3.1 Global chemiluminescence

The study is limited to two chemiluminescent species, OH\* and CH\*. OH\* is measured at a wavelength of 308 nm and CH\* is measured at a wavelength of 431 nm. The voltage measurement is first corrected for wavelength dependent inefficiencies of system components, namely the monochromator grating and the PMT photocathode. (see Section 4.2.1) The corrected voltage measurement is then scaled using the appropriate integrand scaling factor calculated in Section 4.2.2. The corrected and scaled voltage measurement is directly proportional to the total chemiluminescence yield, regardless of the experimental condition or the wavelength of measurement. The proportionality depends only on the burner type and specific optical system configuration used in the measurement. Measurements that have been corrected in this manner will carry units of (cV-A) for 'corrected voltage x Angstroms'. (1 Angstrom (A) = 0.1 nm)

### 4.3.2 Local Chemiluminescence Measurements

Local chemiluminescence studies are limited to the same two chemiluminescent species, OH\* and CH\*. The voltage measurements are corrected exactly like global

chemiluminescence measurements. The optical system configuration used is however very different, so that the quantitative validity of local chemiluminescence measurements is not strictly given. Since local chemiluminescence measurements are at this time only used for illustrative purposes, the lack of a quantitative basis for these measurements is not considered problematic. It is important to mention that the applied correction should allow local comparisons of  $\text{OH}^*$  chemiluminescence to  $\text{CH}^*$  chemiluminescence.