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Sensitivity of the Opal Instrument for Gravity Wave Detection

Kenneth I. Zia
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SENSITIVITY OF THE OPAL INSTRUMENT FOR GRAVITY WAVE DETECTION

by

Kenneth I. Zia

A thesis submitted in partial fulfillment
of the requirements for the degree
of
MASTER OF SCIENCE
in
Physics

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2018
ABSTRACT

Sensitivity of the OPAL Instrument for Gravity Wave Detection

by

Kenneth I. Zia, Master of Science
Utah State University, 2018

Major Professor: Ludger Scherliess, PhD
Department: Physics

Understanding the Earth’s lower thermosphere (altitude range 80-140 km) is of high interest to the space science community because of competing forcing due to solar heating from above and episodic wave forcing from below. The NSF sponsored OPAL (Optical Profiling of the Atmospheric Limb) mission is designed to measure the temperature profile in this region by observing day-time integrated line of sight of the $O_2$ A-band ($\sim 760$nm) emission on the limb. The OPAL instrument, on a 3U CubeSat (10 cm x 10 cm x 30 cm), has an altitude resolution of about 1km at tangent altitudes between 80-140 km and is expected to be launched from the International Space Station (ISS) ($\sim 400$ km altitude). To investigate the instruments ability to detect space weather signatures (i.e. solar storms and gravity waves) in the lower thermosphere, A-band emission data we have developed a suite of models that simulate the flight track of the satellite, the attitude of its optical systems, as well as the expected atmospheric $O_2$ A-band observations that will be seen by the instrument. These models combine in a virtual CCD image that is used to develop and test different OPAL running modes for gravity wave detection. We will present development and integration of the models that resulted in thresholds for gravity wave observations by OPAL.

(69 pages)
PUBLIC ABSTRACT

Sensitivity of the OPAL Instrument for Gravity Wave Detection

Kenneth I. Zia

Knowing what goes on in the upper atmosphere (∼80-140 km) is very important to the space science community. There are several competing forces that influence the temperature and densities of neutral molecules in that region. OPAL (Optical Profiling of the Atmospheric Limb) is funded by the National Science Foundation (NSF) to measure the temperature there using light from oxygen molecules (∼760 nm). To accomplish this, OPAL is built into a CubeSat (a satellite the size of a loaf of bread) to be launched from the International Space Station (ISS) at an altitude of about 400 km. This vantage point is needed to see the light that is absorbed before it makes it to the ground, so a satellite is the optimal choice. Similar to looking at a tennis ball in your hand and trying to see the details of the yellow fuzz fibers on the outer edges of the ball, OPAL is trying to see the light emitted from oxygen at the outer edge of the atmosphere (also called the limb). In order to see how well OPAL can detect space weather signatures affecting the oxygen emissions a suite of models are made to simulate its output. This suite is made of: simulating the flight path of CubeSat, modeling where the OPAL instrument is looking, and how the oxygen light changes with where the instrument is looking. Because we are currently in a solar minimum, the occurrence of solar storms and geomagnetic storms are considered rare events. This allows for the concentrating on detecting gravity waves in this region and the minimum values of detecting them with this developed model.
ACKNOWLEDGMENTS

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1.1 Earth’s Atmosphere

Earth’s atmosphere can be divided into four regions that range from the surface of the Earth to hundreds of kilometers high. The classification of these regions is depicted in Figure 1.1, and is characterized by changes in the average temperature profile gradient associated with each region. The troposphere is the lowest layer from the ground up to about 10 km altitude where a temperature gradient of approximately -7K/km is found. Transitioning from the troposphere to the stratosphere we find the tropopause, where the temperature gradient changes from negative to positive. In the stratosphere from about 10 to 50 km altitude a positive temperature gradient is found due to solar UV absorption by ozone. Above the stratopause, near 50 km altitude, we find another region of gradient inversion that leads into the mesosphere, the coldest region of the atmosphere. Due to radiative cooling, temperatures in this region are \(~130-190\) K. Above the mesosphere is the thermosphere with the largest temperature gradient from absorption of extreme UV and UV radiation. In addition to radiation, there are processes from lower regions and particle precipitation that contribute to the thermal balance of the thermosphere. The dissipation of atmospheric waves, auroral particles from the magnetosphere, and solar protons ejected from the Sun deposits energy. Alternatively, particle precipitation from the magnetosphere at high latitudes causes cooling by altering the chemical composition of the lower thermosphere [Sinnhuber et al., 2012]. These temperature changes can propagate up to the orbit of the International Space Station (ISS) (\(~400\) km altitude) affecting its drag [Solomon, 2000]. The lower thermosphere (\(~90-140\) km) has proven to be a difficult region to study due to minimal data and the large amount of dynamic processes involved.
Figure 1.1: Average atmospheric temperature profile showing regions of the neutral atmosphere. Neutral temperatures from the MSIS empirical model during high solar activity (F10.7 of 200) at mid-latitudes with Summer (red) and Winter (blue). Also shown are the atmospheric regions based on their altitude gradients.

1.2 OPAL Mission

Scarcity of data in the lower thermosphere has led to the term “thermospheric gap” coined by Oberheide et al. [2011]. The OPAL mission objective is to observe the \( \text{O}_2 \) A-band emissions to obtain altitudinal temperature profiles in the “thermospheric gap” region as depicted in Figure 1.2. The A-band is one of the strongest emission features observed in the near infrared region of the airglow spectrum. However, it is prone to strong self absorption below \( \sim 70 \) km altitude which prevents ground-based observations from being made but makes OPAL and other spaced-based remote sensing of this emission more viable. Figure 1.3 shows a log-plot of the molecular oxygen density vs altitude. Because density is proportional to the absorption the exponentially lower density at higher altitudes allows for considerably less self-absorption from above than below the lower thermosphere. Note that an increase in the altitude by 20 km approximately lowers the density of \( \text{O}_2 \) by an order of magnitude in this region.
Figure 1.2: An average plot of temperatures (K) vs altitude (km) with depiction of OPAL’s region of interest. On the right of the temperature profile is a model of the OPAL CubeSat with deployed solar panels (blue rectangles) and image baffle (underneath in black).

Figure 1.3: $O_2$ densities shown as a function of altitude from the MSIS-E 90 global empirical model.
OPAL is following other highly successful temperature observations in the same region; Thermosphere, Ionosphere, Mesosphere Energetics and Dynamics (TIMED) mission with the Sounding of the Atmosphere using Broadband Emission Radiometry (SABER) instrument, Optical Spectrograph and IfraRed Imager System (OSIRIS) mission, and Remote Atmospheric and Ionospheric Detection System / Near IR Spectrometer (RAIDS/NIRS) instrument on the ISS. RAIDS was a pioneering mission for OPAL because it used the same $O_2$ A-band emission but scanned over a smaller altitude range. The OSIRIS and TIMED/SABER also measured the temperature profiles, using different emissions, but their observations were also limited to lower altitudes (below $\sim 110$ km). OSIRIS’s observations and analysis can be found in Sheese et al. [2010], TIMED/SABER observations and analysis are in Mertens et al. [2001], and RAIDS observations and analysis are available in Christensen et al. [2012]. OPAL will build upon the success of these missions using a hyper-spectral imager and a larger altitude range of observations.

1.2.1 OPAL Instrument

The OPAL cubesatellite is developed and built by the Space Dynamics Lab (SDL) and Utah State University (USU) with the intent to study the lower thermosphere. Other missions have observed this region of the upper atmosphere, but OPAL is one of the first hyper-spectral imagers on a CubeSat. These other missions observed emissions at the atmospheric limb to observe the dynamics of the lower thermosphere, similar to OPAL’s mission. However, the hyper-spectral imager of OPAL allows for a full spectrum image of OPAL’s entire field of view (FOV) simultaneously. This is preferred to the method of scanning across the limb altitudinally to investigate spectrum’s vertical profile, which causes a time delay between measurements. Figure 1.4 shows the details of the spectral imager with the path light takes from the limb to the focal plane array which is a charge coupled device (CCD). The components distinct to this instrument are the 7-slit array between the lens groups 1 and 2 and the volume holographic grating (VHG) between lens groups 2 and 3. The slit array is used to divide the horizontal FOV at 350 km into seven equal regions that are imaged by each slit as shown in Figure 1.5. These slit images are then diffracted
from the VHG to split the slit images into their spectral components with only the $\sim 762 \text{ nm}$ wavelengths of $O_2$ emissions spread onto the CCD. Details of the instrument’s capabilities are shown in Table 1.1.

**Figure 1.4:** Diagram of the OPAL instrument optical setup. Rays trace light from the atmospheric emission to the focal plane array (FPA) (adapted from Marchant et al. 2014).

**Figure 1.5:** Depiction of how the slits split the full field of view into seven regions and how the volume holographic grating spreads the signal into wavelength components onto the focal plan array.
### Table 1.1: OPAL Instrument Capabilities [Marchant et al., 2014].

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<th>Parameter</th>
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<tbody>
<tr>
<td>Vertical FOV</td>
<td>80-160 km</td>
</tr>
<tr>
<td>Vertical Resolution</td>
<td>1.03 km, 0.033°</td>
</tr>
<tr>
<td>Horizontal FOV</td>
<td>10°</td>
</tr>
<tr>
<td>Horizontal Resolution</td>
<td>1.7°</td>
</tr>
<tr>
<td>7-slit array</td>
<td>3.00 x 0.05 mm</td>
</tr>
<tr>
<td>Spectral Resolution</td>
<td>0.50 nm</td>
</tr>
<tr>
<td>Holographic Grating</td>
<td>1540 lpmm</td>
</tr>
<tr>
<td>CCD Quantum Efficiency</td>
<td>50%</td>
</tr>
<tr>
<td>CCD Well Capacity</td>
<td>23,000 e-</td>
</tr>
<tr>
<td>Readout Noise</td>
<td>5 e- rms</td>
</tr>
<tr>
<td>Readout Rate</td>
<td>60 frames/s</td>
</tr>
<tr>
<td>Dark Current</td>
<td>0.1 e-/s at 10° C</td>
</tr>
</tbody>
</table>

#### 1.2.2 Science Goals

One of OPAL’s science goals is to observe the thermospheric response to energy inputs on a global and regional scale. Geomagnetic storms are one of the most prevalent energy inputs in the higher latitudes and causes increases in thermospheric temperatures. Although OPAL is expected orbit at the ISS’s inclination (51.6 degrees latitude), making it incapable to observe direct effects of solar storms at high latitudes, it could give needed insight into the thermal response of the energy transport to low and mid-latitudes. Solar flares are also an external energy source is not localized to one latitude range, but effects the entire day-side of the atmosphere. The energy transport and thermal response at lower latitude are modeled by the Thermosphere Ionosphere Electrodynamics Global Circulation Model’s (TIEGCM) simulated temperature response to a solar flare. Figure 1.6 shows this response at near equatorial latitude [Qian et al., 2010]. Figure 1.6 also shows that there is a possible 0.5% to 2.0% observable change in the thermospheric temperature profile over OPAL’s vertical field of view. Observations of this effect are capable with OPAL, and improved from previous missions by the instrument’s extended altitude range above 110 km [Wilson et al., 2006].

The second main science goal of OPAL is studying the internal forcing of the lower
thermosphere by atmospheric waves. Atmospheric waves comprise temporal and spatial scale-based categories. The largest scale waves are planetary waves (also known as Rossby waves) that are global scale waves with horizontal wavelengths on the order of thousands of kilometers. They are currently thought to be produced by strong winds blowing over large mountain ranges or large heating differences between continents and oceans. Next largest scale are atmospheric tides which are produced from solar UV radiation heating the stratospheric ozone and tropospheric water vapor. Because they are generated from solar radiation, they are on a global scale with wavelengths ranging in several thousands of kilometers and typically propagate with the sun-side of the Earth. The smallest category are the atmospheric gravity waves which are generated by processes in the troposphere: tropospheric wind over mountain ranges, latent heat release from convective regions, or jet stream shear. Fritts and Alexander [2003] describes the physical parameter of gravity waves’ vertical wavelength as being on the scale of kilometers to tens of kilometers and their horizontal wavelengths from tens to hundreds of kilometers. Both types of waves, traveling from low to high altitudes, are a key pathway for momentum and energy flowing into the lower thermosphere. This becomes a major driver for thermospheric variability during quiet solar conditions. An example gravity wave observation is shown in the top panel of Figure 1.7 where a Lidar in the South Pole observed harmonic perturbations in
Figure 1.7: Lidar measurements on 28 May 2011, McMurdo, Antarctica, showing a gravity wave temperature perturbation of period 1.5-2 hr in the OPAL observation region. (adapted from Chu et al. [2011]).

the iron density on the vertical scale of a gravity wave [Chu et al., 2011]. The bottom panel shows the perturbations in the temperature profile. The vertical structure of the underlying wave can be determined by comparing to a background profile (the dashed line in the plot), which is an averaged temperature profile from the MSIS00 model. OPAL’s analysis will improve on the database background by producing an average made from its own measurements to produce a background.

1.3 Thesis Objective

This thesis focuses on the viability of the second science goal, atmospheric wave detection, with OPAL’s expected launch in the solar minimum where the wave detection is maximized with minimal energy forcing from above.
CHAPTER 2
A-BAND EMISSIONS

2.1 Introduction

Understanding the spectrum of molecular oxygen in the atmosphere comes from considering the structure of its three lowest electronic states. These states are: the ground state $O_2(X^3\Sigma)$, the first excited electronic state $O_2(a^1\Delta)$, and the second excited electronic state $O_2(b^1\Sigma)$. Each of these electronic states has vibrational levels ($v$), and transitions between the vibrational states giving a wide range of absorption and emission lines as seen in Figure 2.1.

![Schematic of electronic states](image)

**Figure 2.1:** From left to right: (0,1) band (emission), $\gamma$-band (absorption), B-band (absorption), A-band (absorption/emission), and the Infrared Atmospheric (0-0) band (absorption/emission).

For OPAL, the transition of interest is the $O_2(b^1\Sigma, v = 0)$ to $O_2(X^3\Sigma, v = 0)$ which is the Infrared Atmospheric (0-0) band emission. This emission corresponds to a wavelength of
about 762 nm, also known as the atmospheric A-band. Figure 2.1 references the transition between the electronic and vibrational states. However, when also accounting for transitions between rotational states an entire spectrum centered about the 762 nm line emerges [Goody and Yung, 1989].

This chapter will first describe the three most relevant atmospheric mechanisms for OPAL that populate the excited state \( O_2(b^1 \Sigma, v = 0) \), and how they combine to give a volume emission rate of the A-band. This will be followed by a discussion of the A-band spectrum and, most importantly to the OPAL mission, its temperature dependence.

2.2 Production of A-band’s Excited State

To calculate the intensity of A-band emission that will be seen by OPAL the population of \( O_2(b^1 \Sigma, v = 0) \) states must be known. For the altitude range of the OPAL observations this excited \( O_2 \) molecule has three production processes which we will consider: the resonant scattering of solar flux, the collision of \( O_2 \) with ionized atoms, and the Barth three body collision.

There are ion contributions to this band of emission but, in this region of the atmosphere the neutral molecular densities are much higher and in this study ionic components are neglected. For the neutral molecules, photochemical equilibrium of chemical reactions is used to describe the production of the \( O_2(b^1 \Sigma, v = 0) \) state. Photochemical equilibrium of the A-band’s excited \( O_2 \) state (\( O_2^* \)) is then represented as \( \frac{d[O_2^*]}{dt} = 0 = Production - Loss \cdot [O_2^*] \), meaning that local density is described as \( [O_2^*] = \frac{Production}{Loss} \), where the production is the three processes being considered. The loss will be discussed when combing them into the total volume emission rate.

2.2.1 Resonance Scattering

The first of the three primary sources of the \( O_2(b^1 \Sigma, v = 0) \) state in the lower thermosphere is photon absorption due to resonant scattering of A-band photons. Figure 2.1 shows three vibrational levels of the \( O_2(b^1 \Sigma) \) state \( (v = 0, 1, 2) \), and each one can be excited
via a separate narrow band of light corresponding to an atmospheric band. For the A-band this corresponds to absorption of 762 nm light through,

\[ P_{\text{res}A} = g_A [O_2] \]  

(2.1)

with \([O_2]\) referring to the number density of ground state \(O_2\) with units of molecules/cm\(^3\). The factor \(g_A\) is the photochemical reaction coefficient with units of \([s^{-1}]\). Following Bucholtz et al. [1986], the g-factor can generally be calculated as,

\[ g(z, \chi) = \int F(\nu, z, \chi) \sum_j S_j(T) D(\nu) d\nu \]  

(2.2)

This factor is a function of altitude and solar zenith angle (\(\chi\)) and is dependent on the solar flux \((F(\nu, z, \chi))\) at wavenumber (\(\nu\)) and altitude (\(z\)), the line strength \((S_j(T))\) as a function of temperature, and the Doppler line shape \((D(\nu))\). Only Doppler broadening is considered because it is the dominant effect above 40 km, which adds a unit less normalized Gaussian distribution about the line \(j\) in the sum of Equation 2.2 [Goody and Yung, 1989]. Making this generalized g-factor into \(g_A\) comes about by integrating the wavenumber (\(d\nu\)) over the A-band’s range of \(~760-770\) nm. Figure 2.2 shows the altitude dependence of \(g_A\) and how it varies with solar zenith angle. In the region of interest, for the OPAL mission, the value of \(g_A\) for different zenith angles converge to a single value of \(6.18 \times 10^{-9} (s^{-1})\) at altitudes above 100 km. However, at OPAL’s lower end, 80 km, only the solar zenith angle of 90 degrees is about 20% from the converging value of the other solar zenith angles at that altitude. Therefore the production of \(O_2(b^1\Sigma, v = 0)\) in Equation 2.1 can be amended to,

\[ P_{\text{res}A} \approx (6.18 \times 10^{-9}) \times [O_2]. \]  

(2.3)

### 2.2.2 \(O(^1D)\) Collisions

The second production of \(O_2(b^1\Sigma, v = 0)\) is a result of collisions between the ground state \(O_2(X^3\Sigma, v = 0)\) and excited atomic oxygen, \(O(^1D)\). The process is shown by
Figure 2.2: Photochemical reaction coefficient, $g_A$, with varying zenith angles as a function of altitude (adapted from Sheese [2009]).

Bucholtz et al. [1986] to be,

$$P_{O(1D)} = \phi k_1 [O(1D)] [O_2]$$  \hspace{1cm} (2.4)

Where $k_1$ is the collisional frequency between the two species, $[O(1D)]$ and ground state $[O_2]$, and $\phi$ is the efficiency of the collisions producing, specifically, the $O_2(b^1\Sigma, v = 0)$ state [Bucholtz et al., 1986].

To compute the rate of this collisional source of A-band’s excited state, the production of $O(1D)$ needs to be calculated because its number density is generally not reported in atmospheric data bases. The primary production of $O(1D)$ results from photodissociation of $O_2$ in the Schumann-Runge Continuum (SRC), the band of wavelengths between 135 and 176 nm, and of $O_3$ in the Hartley Band, wavelengths between 200 and 300 nm, by solar ultraviolet radiation. This production can be represented as

$$[O(1D)] = J_2[O_2] + J_3[O_3],$$  \hspace{1cm} (2.5)
with the photolysis coefficients $J_2$ and $J_3$ being the rates at which photodissociation occurs for the $O_2$ and $O_3$ respectively.

Similarly to the $g_A$ coefficient, the $J_2$ and $J_3$ coefficients are dependent on solar flux, altitude, and solar zenith angle. Following Brasseur and Solomon [2006], this can be expressed as

$$J(z) = \int F(\lambda, z)\sigma(\lambda)\phi d\lambda,$$

Equation 2.6 is comprised of solar flux ($F(\lambda, z)$) with units of photons/(s*cm$^2$), absorption cross-section ($\sigma(\lambda)$) with units of cm$^2$/molecule, and the quantum yield ($\phi$) with units of molecules/photon. The molecular absorption cross-section area for $[O_2]$ and $[O_3]$ is constant over the respective photodissociation UV bands. The $J_3$ value for altitudes over 70 km and solar zenith angles less that 85 degrees is numerically calculated by Sheese [2009] to be $7.1 \times 10^{-3}$[s$^{-1}$]. $J_2$ is shown for different solar zenith angles as a function of altitude in Figure 2.3(a), and Figure 2.3(b) is a function to approximate $J_2$ to three orders of magnitude, 140-100 km altitude, at a solar zenith angle between the 0 and 90 degree angle. With $J_2$ and $J_3$ defined, the production of $O(^1D)$ is understood, but there are processes that can attribute to loss of $O(^1D)$ before it excites $O_2$ to the A-band excited state.

\begin{figure}[h]
\centering
\begin{subfigure}{0.45\textwidth}
\centering
\includegraphics[width=\textwidth]{figure_a}
\caption{(a)}
\end{subfigure}
\begin{subfigure}{0.45\textwidth}
\centering
\includegraphics[width=\textwidth]{figure_b}
\caption{(b)}
\end{subfigure}
\caption{(a) Photolysis coefficient, $J_2$, plotted by solar zenith angle as a function of altitude (adapted from Sheese [2009]). (b) $J_2$ as a function of altitude to an approximated solar zenith angle between 90 and 0 degrees ($J_2(z) = 6.0 \times 10^{-10}z^2 - 1.0 \times 10^{-7}z + 4.0 \times 10^{-6}$).}
\end{figure}
There is a loss component considered for the production of \([O(1D)]\) that must be the divisor of the production terms to produce a more accurate production rate. This loss is due to collisions that quench the excited oxygen atom before it can produce \(O_2(b^1\Sigma, v = 0)\).

\[
[O(1D)] = \frac{J_2[O_2] + J_3[O_3]}{A_{1D} + k_1[O_2] + k_2[N_2]}
\]  

(2.7)

Here the collisions with \([O_2]\) and \([N_2]\) de-excite the \(O(1D)\) at collision rates of \(k_1\) and \(k_2\) respectively. There is also sporadic decay from the excited \(O(1D)\) to the lower \(O(3P)\) at a rate dictated by the Einstein coefficient \(A_{1D}\). The decay of \(O(1D)\) to \(O(3P)\) produces radiation at 630 nm which is well outside of the A-band and OPAL measurement spectrum \[Streit et al., 1976\].

Using Equation 2.7 to substitute the \([O(1D)]\) into Equation 2.4,

\[
P_{O(1D)} = \frac{\phi k_1(J_2[O_2] + J_3[O_3])[O_2]}{A_{1D} + k_1[O_2] + k_2[N_2]}
\]  

(2.8)

gives the complete equation for production of \(O_2(b^1\Sigma, v = 0)\) through the \(O(1D)\) process.

2.2.3 Barth Process

The Barth process is the last mechanism considered for production of the state \(O_2(b^1\Sigma, v = 0)\). The Barth process uses a two step process of the three body collision of two oxygen atoms,

\[
O + O + M \rightarrow O_2^* + M
\]  

(2.9)

\[
O_2^* + O_2 \rightarrow O_2(b^1\Sigma, v = 0) + O_2
\]  

(2.10)

\(O\), and a neutral molecule, \(M\) (i.e. \(N_2, O_2\ldots\)), to produce an unstable (decays quickly compared to other states in these processes) excited state of molecular oxygen, \(O_2^*\), which is described by Equation 2.9 \[Bucholtz et al., 1986\]. The second step, shown in Equation 2.10, is the two body collision of the unstable excited oxygen molecule, \(O_2^*\), with an oxygen
molecule at a lower energy level to produce the molecular state of interest, $O_2(b^1\Sigma, v = 0)$. These collisions are represented in the Barth production Equation 2.11, which also includes $O^*$ loss, by McDade et al. [1986],

$$P_{Barth} = \frac{k_5[O]^2[O_2][M]}{C_{O_2}[O_2] + C_O[O]} \quad (2.11)$$

The denominator is, again, the loss term associated with excited $O_2^*$ colliding with $O_2$ to produce an undesirable state of $O_2$ at a rate coefficient of $C_{O_2}$. The other part of the loss term is through $O_2^*$ collisions with $O$, instead of $O_2$, at a rate coefficient of $C_O$. The rate at which this three body process occurs, $k_5$, is derived from Campbell and Gray [1973] and is the smallest rate coefficient by several orders of magnitude at $10^{-33}$. Thus making the Barth process the smallest contributor of the production of $O_2(b^1\Sigma, v = 0)$.

### 2.3 Volume Emission Rate

The three prominent mechanisms’ production of the excited state of A-band emission, $O_2(b^1\Sigma, v = 0)$, were shown to be produced by resonant A-band scattering, $O(^1\text{D})$ collision, and the Barth process. They are summed together to give the total number density of $O_2(b^1\Sigma, v = 0)$ in a region. This sum is then made into another production/loss equation for the volume emission rate of the A-band emission,

$$\nu = F_C \frac{A_{1\Sigma}(P_{resA} + P_{O(^1D)}) + P_{Barth}}{A_{1\Sigma} + k_0[N_2] + k_3[O_3] + k_4[O_2] + k_6[O]} \quad (2.12)$$

The overall production of A-band emission is determined by the rate that the $O_2(b^1\Sigma, v = 0)$ state decays to the $O_2(X^3\Sigma, v = 0)$, which is given by another Einstein coefficient, $A_{1\Sigma}$. Loss terms are also considered as collisional rates of the excited $O_2(b^1\Sigma, v = 0)$ with other neutral molecules and atomic oxygen, and the Einstein coefficient is also considered as a loss factor. Lastly, there is the Franck-Condon factor, $F_C$ for the A-band which is the transition probability between the two $v = 0$ states of $O_2$ to produce A-band emission derived from Nicholls [1965]. This division of production by loss terms combine, Equation 2.12, to define the volume emission rate of the (0,0) A-band in units of photons/s/cm$^3$ [Sheese,
All reaction coefficients used are defined in Table 2.1. The results of this analysis is shown in Figure 2.4 with the breakdown of each constituent process shown in different colors. Figure 2.4 is produced from the MSIS-E 90 (Mass Spectrometer and Incoherent Scatter) model’s neutral temperature and neutral densities ($O, N_2$, and $O_2$) on July 19th 2015 at 13.5 UT over Logan, UT [Hedin, 1987]. The only value not from this database was the ozone density that is from averaging SABER ozone profiles from July 2004 to achieve a typical summer profile from Sheese [2009]. As mentioned in the Barth process, the rate coefficient was the weakest by several orders of magnitude and is shown to peak at a magnitude of $10^3$ while the other processes have peaks in $10^4$. The $O(1D)$ is divided into its two main productions of photodissociation of $O_2$ and $O_3$. The curve for $O_3$ is the shape of its density curve as it is weighted by a constant, while the $O_2$ curve is weighed heavily by the $J_2$ coefficient at the lower altitude of the function which is cut off at 100 km to prevent negative values of the approximated function from skewing the total emission. The blue line is the resonant scattering production and represents the $O_2$ density profile weighed by the constant A-band g-factor.

![Figure 2.4](image)

**Figure 2.4**: The total volume emission rate of the A-band shown with each process inputted given in a different color. This volume emission rate is specific to that latitude, longitude, time of day and year as a function of the neutral temperature and densities given from the MSIS-E 90 database. The $O(1D)$ process is broken into the $O_3$ and $O_2$ components to show the dependence on the $O_3$ and $O_2$ densities in the lower thermosphere.
Table 2.1: Coefficients of Reactions for the Production of the A-band (Units [s⁻¹]).

<table>
<thead>
<tr>
<th>Rate Constant</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_{1\Sigma} )</td>
<td>0.085</td>
<td>Burch and Gryvnak 1969</td>
</tr>
<tr>
<td>( A_{1D} )</td>
<td>6.81(-3)</td>
<td>Kernahan and Pang 1975</td>
</tr>
<tr>
<td>( A_{771} )</td>
<td>0.070</td>
<td>Yankovsky and Manuilova 2006</td>
</tr>
<tr>
<td>( C_O )</td>
<td>0.085</td>
<td>McDade et al. 1986</td>
</tr>
<tr>
<td>( C_{O2} )</td>
<td>7.5</td>
<td>McDade et al. 1986</td>
</tr>
<tr>
<td>( F_C )</td>
<td>0.93</td>
<td>Nicholls 1965</td>
</tr>
<tr>
<td>( g_A )</td>
<td>6.18(-9)</td>
<td>Bucholtz et al. 1986</td>
</tr>
<tr>
<td>( J_2 )</td>
<td>See Text</td>
<td>Sheese 2009</td>
</tr>
<tr>
<td>( J_3 )</td>
<td>7.1(-3)</td>
<td>Sheese 2009</td>
</tr>
<tr>
<td>( k_0 )</td>
<td>1.8(-15)exp(45/T)</td>
<td>Sander et al. 2006</td>
</tr>
<tr>
<td>( k_{0B} )</td>
<td>4.5(-11)exp(-312/T)</td>
<td>Yankovsky and Manuilova 2006</td>
</tr>
<tr>
<td>( \phi )</td>
<td>0.95</td>
<td>Green et al. 2000</td>
</tr>
<tr>
<td>( k_1 )</td>
<td>3.3(-11)exp(55/T)</td>
<td>Sander et al. 2006</td>
</tr>
<tr>
<td>( k_2 )</td>
<td>2.15(-11)exp(110/T)</td>
<td>Sander et al. 2006</td>
</tr>
<tr>
<td>( k_{2B} )</td>
<td>5(-13)</td>
<td>Yankovsky and Manuilova 2006</td>
</tr>
<tr>
<td>( k_3 )</td>
<td>3.5(-11)exp(135/T)</td>
<td>Sander et al. 2006</td>
</tr>
<tr>
<td>( k_{3B} )</td>
<td>3(-10)</td>
<td>Yankovsky and Manuilova 2006</td>
</tr>
<tr>
<td>( k_4 )</td>
<td>3.9(-17)</td>
<td>Sander et al. 2006</td>
</tr>
<tr>
<td>( k_5 )</td>
<td>4.7(-33)exp(300/T)²</td>
<td>Campbell and Gray 1973</td>
</tr>
<tr>
<td>( k_6 )</td>
<td>8(-14)</td>
<td>Sander et al. 2006</td>
</tr>
</tbody>
</table>

2.4 A-band Spectra

As described in this chapter’s introduction, there are two electronic states of interest; the ground state \( O_2(X^3\Sigma, v = 0) \) and the second excited electronic state \( O_2(b^1\Sigma, v = 0) \). There are also rotational levels of \( O_2 \)’s states designated by quantum numbers \( K, S, \) and \( J \) of the molecule, where \( K \) represents rotational angular momentum, \( S \) is the total electron spin, and \( J \) is the total angular momentum.

\[
J = K + S \tag{2.13}
\]

Developing the spectrum of the A-band requires transitions between the total angular momentum states of the excited and ground state. Spectroscopy defines these possible transitions as branches that correspond to changes in rotational angular momentum \( (\Delta K) \) within the transition of the electronic state. There are three spectral branches present in the A-band, \( \Delta K = 1, 0, -1 \) as the P branch, Q branch, and R branch respectively. There
are higher order branches possible in other transition, but it will be seen that the A-band
only has P and R branches possible in its spectrum [Herzberg and Herzberg, 1947].

The dominant isotope of oxygen is $^{16}O_2$, and it is the only homonuclear diatomic
molecule of the three naturally occurring isotopomers; meaning this isotope of $O_2$ has a
nucleus of zero nuclear spin. This property allows for the two valence electrons’ spin (mag-
netic moment) to dominate the interactions between them. These interactions come into
effect when considering possible total angular momentum and electronic spin of the oxygen
molecule [Gamache et al., 1998]. Considering the electronic ground state $O_2(X^3Σ, v = 0)$,
it has integer electron spin $S = 1$. This integer spin has coupling of electronic spin and
angular momentum which allows for a triplet of states in total angular momentum, $J$;
$J = K + 1, J = K, J = K - 1$. The integer spin of the ground state is associated with
the electrons’ total wavefunction to be antisymmetric about the center of the molecule and
results in only odd rotational angular momentum ($K$) states allowed. The excited state
$O_2(b^1Σ, v = 0)$ has a total spin of $S = 0$, and results in a singlet of $J$ in which $J = K$
(rotational angular momentum is the total angular momentum). This state has a symmetry
of the electrons’ total wavefunction about the center of the molecule that allows only even
$K$ states to be populated [Schlapp, 1932].

With $K$ states in the excited level restricted to even and the ground level restricted to
even, there is no change in $K$ states ($ΔK$) that can equal zero and therefore no possible
Q branch for the A-band. The P and Q branches are further divided through possible
transitions from the excited $J = K$ states to the ground state’s triplet of $J$ states. This is
denoted with $ΔK ΔJ$ with $ΔK$ only able to be P or Q as the main branch and $ΔJ$ for sub-
branches of the possible transitions to the triplet states. Figure 2.5 shows the excited state’s,
$O_2(b^1Σ, v = 0)$, even angular momenta and their allowed transitions into the ground state’s,
$O_2(X^3Σ, v = 0)$, triplet angular momenta as discussed by the symmetry/antisymmetry of
each state. This figure also shows that the first transition is a $P P$ transition, skipping over
the expected $P Q$ from $J = 0$ singlet to $J = 0$ of the triplet. This is due to magnetic dipole
interaction selection rules. The magnetic dipole interaction is evident in the integer spins
of the electrons in each state, and therefore must obey the exclusion of transitions from a $J = 0$ state to a $J = 0$ state derived from the transition moment integral \cite{Harris and Bertolucci, 1978}.

Figure 2.5: Depiction of spectroscopic branches possible in the transitions of the A-band electronic states.

As seen in Figure 2.5 there are four types of transitions allowed from each of the excited $J$ states, except $J = 0$; the $P^P$, $P^Q$, $R^R$, $R^Q$. Each of these branches have an intrinsic relative strength that is derived in Schlapp \cite{1937} by solving the Hamiltonian for the integer spin states and decoupling the spin. This derivation results in the intensity of each transition line, $i$, as a function of $J$, total angular momentum for each branch,

\begin{align}
  i^{(P^P)} &= \frac{1}{2} (J + 2); & i^{(P^Q)} &= \frac{1}{2} \left( J + \frac{3}{4} \right); & i^{(R^R)} &= \frac{1}{2} (J - 1); & i^{(R^Q)} &= \frac{1}{2} \left( J + \frac{1}{4} \right). \\
  (2.14)
\end{align}

This equation has each excited $J$ state’s relative line intensities defined. These relative intensities are then applied to statistical mechanics to determine a temperature ($T$)
dependence. Because of the integer spin’s bosonic behavior of the upper and lower states Bose-Einstein statistics can be used to find the probability of angular momentum excited states being populated by the electrons. This technique is used to obtain Equation 2.15 to weight each line’s excited angular momentum state’s population probability to get temperature dependent line strength ($S(J, T)$).

$$S(J, T) = i(J) \cdot \exp \left( \frac{-hcE_J}{k_BT} \right)$$  \hspace{1cm} (2.15)

Here $k_B$ is the Boltzmann constant, $E_J$ is the energy of the excited state’s $J$ state, $h$ is Planck’s constant, and $c$ is the speed of light. To apply these line strengths there needs to be an associated wavelength or frequency to form the spectrum. This is defined by the total energy difference between the excited energy transition to the ground energy level. These energy levels are including the energy of the total angular momentum of those states.

$$\kappa(J) = \nu + F\nu_{Upper} - F\nu_{Lower}$$  \hspace{1cm} (2.16)

$\kappa(J)$ is the wavenumber of that transition and can be converted to wavelength, $\lambda(J)$.

### 2.4.1 Temperature Dependence Analysis

Together, $S(J, T)$ and $\lambda(J)$ are used to make the temperature dependent spectrum shown in Figure 2.6; where the smaller wavelength grouping is the R-branch, the P-branch is the longer wavelength grouping, and the missing lines around 762 nm are the absent Q-branch from this transition. The 200 K plot, Figure 2.6(a), compared to the 296 K plot, Figure 2.6(b), shows a narrowing of the R-branch and a broadening of the P-branch, and an overall decrease in line strength at the higher temperature as the strengths shift to longer wavelengths. The same features of 200-296 K are intensified in comparison to the 800 K plot, Figure 2.6(c), with much more narrowing of the the R-branch, broadening of the P-branch, and half the line strengths of the 200 K at the peaks of the branches (0.04 to 0.02 of the R-branch lines peaks).
Figure 2.6: A-band temperature dependent spectrum line strength analysis. (a) 200 K plot of A-band spectrum, (b) 296 K, standard temperature, and (c) 800 K plot of A-band spectrum.
A clarification must be made between the transmission band that has been derived in this chapter and the absorption band given from the HITRAN (HIgh-resolution TRANsmission molecular absorption) Database. There are two main differences between the line strengths of the derived A-band, Figure 2.6, and the HITRAN strengths, Figure 2.7: the strongest lines of either branch are in the R-branch of HITRAN and the P-branch of the A-band, and the number of lines is much larger in HITRAN (486 lines) vs. A-band (165 lines) which is limited to $^{16}\text{O}_2$ isotope. Switching which branch is the strongest could lead to issues in obtaining accurate temperatures from the data in processing. The extra lines of HITRAN is not a concern, even though it uses less populous isotopes of $\text{O}_2$, the other isotope’s lines are weighted by the relative density compared to the $^{16}\text{O}_2$. This weighing by population puts the extra lines well below the most common lines as seen in the Figure 2.7.

![Figure 2.7](image)

**Figure 2.7:** $\text{O}_2$ absorption temperature dependent spectrum line strength analysis. (a) 200 K plot of $\text{O}_2$ absorption spectrum, (b) 296 K, standard temperature, and (c) 800 K plot of $\text{O}_2$ absorption spectrum.
3.1 Introduction

To produce a simulation of the observations that OPAL will make, there are two important aspects of the instrument that must be understood: the orientation of the OPAL instrument and temporal integration of emission. Chapter 1 has the specifications of the instrument and how the information from the limb is gathered. This chapter’s focus is on only the center of the seven imaging slits of OPAL for clarity of the analysis, but the full field of view will be used for later analysis.

3.2 Orientation of the Instrument

Analyzing OPAL’s orientation is essential in simulating its measurements of the lower thermosphere where parameters change according to the geophysical condition, local time and position around the globe. The orbital dynamics of OPAL is modeled using Analysis Graphics Inc.’s (AGI) System Tool Kit (STK) using the orbital parameters of the International Space Station (ISS). The software’s output was Earth-centered Earth-fixed (ECEF) Cartesian coordinates of position and velocity in time steps of one second. Next the ECEF coordinates are translated into ellipsoid Earth spherical coordinates. Using the World Geodetic System 1984 (WGS84) model to produce latitude, longitude, and altitude coordinates for the cubesat’s position. The parameters associated with the WGS84 model and an example coordinate conversion are given in Table 3.1. With the use of STK’s output and the coordinate transformation, Figure 3.1 shows an example of one orbit of OPAL at the same altitude and inclination of the ISS, with arrows showing the tangent of its orbit along the direction of motion.

Following the position of OPAL, the line of sight (LOS) of the instrument is created with
an Earth-ward pitch of $\theta = 17.728^\circ$ from the orbit’s tangent (demonstrated in Figure 3.3).

The velocity output from STK is used as the tangent vector of OPAL’s orbit. This tilt gives a tangent point altitude in the LOS of 80 km. This is numerically accomplished through the Rodrigues’ rotation formula [Brockett, 1984],

$$
\vec{V}_{\text{Rotation}} = \vec{V} \cos(\theta) + (\vec{K} \times \vec{V}) \sin(\theta) + \vec{K} (\vec{K} \cdot \vec{V}) (1 - \cos(\theta))
$$

(3.1)

where $\vec{V}_{\text{Rotation}}$ is a vector that points along the LOS, $\vec{V}$ is the direction of motion of OPAL, and $\vec{K}$ is a vector normal to the plane of velocity vector $\vec{V}$, and the position vector, $\vec{R}$ (Seen in Figure 3.2).

$$
\vec{K} = \vec{V} \times \vec{R}
$$

(3.2)

### 3.3 Virtual CCD

To integrate the A-band emission to the instrument, the LOS to the tangent point and FOV are used to define the instrument’s orientation. The volume emission rate (‘$\nu$’ of Equation 2.12 derived in Chapter 2) is integrated in 1 km steps along the LOS and summed down the center, right, and left side and averaged together for each slit’s FOV at each
tangent altitude. Each of these steps along the LOS has the volume emission rate evaluated for that latitude’s, longitude’s, and altitude’s molecular densities and temperature at that time step. The MSIS-E 90 empirical model is given latitude, longitude, altitude, local time, and solar cycle obtain the neutral temperature, number densities of $O, N_2$, and $O_2$ used in calculating the volume emission rate [Hedin, 1987]. To integrate the expected intensity $[\text{photons s}^{-1} \text{cm}^{-2}]$ of a single LOS onto the detector,

$$LOS_{I\lambda} = \sum_{\text{step}=0}^{4000} \nu \cdot S_{\lambda} \cdot \Delta x$$

(3.3)

This equation of line of sight integration (LOSI) takes the intensity of each line of the A-band emission and integrates it over the step size, $\Delta x$, of 1 km. $\nu$ is the total emission of the region based off neutral densities and temperature, and is weighted by the temperature dependent line strengths.

### 3.3.1 Signal Integrating

The integration time for the OPAL instrument is set at 30 seconds. This time was used to increase the signal to noise ratio (SNR) of signal from higher altitudes; where the emission are orders of magnitude weaker. A high SNR is needed to obtain the full temperature profile to observe the changes due to large solar effects in the lower thermosphere. The signal, proportional to Figure 2.4, is a full two orders of magnitude smaller at the top of OPAL’s vertical FOV than the bottom. The higher altitude SNR is needed to observe the effects of geomagnetic storms and solar flares on the thermospheric temperature profile. However, when approaching the atmospheric wave science goal of OPAL there are two parameters

![Figure 3.2: Depiction of Rodrigues’ rotation vectors.](image)
to consider. The vertical wavelength of the waves varies spatially from a few to tens of kilometers and the horizontal wavelengths can range from tens to thousands of kilometers \cite{Fritts_and_Alexander, 2003}. To maintain the integrity of the waves in the signal of OPAL, a shorter integration time is necessary to preserve the wave signature. This is at the cost of reduced signal to noise at higher altitudes.

The final step in the model for OPAL’s output is to take the integrated signal from each LOS, and convert it to a pixel row on the CCD. Horizontally on the CCD as seen in Figure 1.5, there is wavelength of the spectrum with each pixel holding 0.5 nm of signal that is binned by a 0.5 nm triangle function. The horizontal bins begin at 750.0 nm and end at 815.0 nm with every 0.5 nm between them as a bin. Beyond that, each slit is represented horizontally with its own spectrum. Vertically, each pixel up is approximately 1 km (1.07 km from the specification Table 1.1 ). Looping through these altitudes and slits in the code produces a full CCD modeled virtually that would represent a one second integration time of the OPAL instrument. Chapter 4 will apply this technique to determine the detect ability of vertical and horizontal wave structures in the atmosphere’s model.
Figure 3.4: Virtual CCD separated by slit image with 1 second integration, with color bar units of photons per second.

Table 3.1: Parameters Used in Calculating WGS84 Coordinates With Example Conversion of Initial OPAL Position.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
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<tbody>
<tr>
<td>Position X</td>
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<td>km</td>
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<tr>
<td>Position Y</td>
<td>319.377</td>
<td>km</td>
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<tr>
<td>Position Z</td>
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<td>Longitude</td>
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<td>deg</td>
</tr>
<tr>
<td>Altitude</td>
<td>401.662</td>
<td>km</td>
</tr>
<tr>
<td>Velocity X</td>
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<td>km/s</td>
</tr>
<tr>
<td>Velocity Y</td>
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<td>km/s</td>
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<tr>
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</tr>
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<tr>
<td>Geocentric Gravitational Constant</td>
<td>3.986(14)</td>
<td>m³/s²</td>
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CHAPTER 4
MODEL SIMULATION AND RESULTS

4.1 Introduction

The goal of this chapter is to test OPAL’s ability to detect small scale perturbations in atmospheric temperature. These perturbations are considered to be caused by gravity waves propagating in the lower thermosphere. Showing detectability is achieved by superimposing wave perturbations on a background thermospheric temperature field and comparing the OPAL specifications of them with the originally imposed structure. The virtual CCD images produced in this chapter are obtained using the initial position and velocity conditions given in Table 3.1 and the instrument resolution parameters shown in Table 1.1.

4.2 Wave Production

Some of the characteristic properties of gravity waves were already described in Chapter 1 but this alone does not describe the effect this has on the atmospheric emission. Williams et al. [2002] describes the temperature changes associated with gravity waves observed using a sodium Lidar over Fort Collins, CO and found waves with associated temperature perturbations of ±50K at a background temperature of 280K. This is an almost 20% perturbation in the temperature; which is believed to be at the higher end of temperature changes due to gravity waves. Even though this is representative of the higher range observed, the model uses the 20%. Furthermore, the initial wave was assumed to propagate only in the vertical direction and have infinite horizontal wavelength. This can be expressed as,

\[ T_{\text{wave}}(z) = T_N(z) \cdot \Delta T \cdot \sin (k_v z) + T_N(z) \]  

(4.1)

Here z is altitude in kilometers, \( k_v \) is the vertical wavenumber defined by \( \frac{2\pi}{\lambda_v} \) (\( \lambda_v \) is the vertical wavelength), \( \Delta T \) is the percentage of temperature perturbation caused by the
wave, and $T_N$ is the atmospheric neutral temperature as a function of altitude. Because the superimposed wave only depends on altitude, it would be analogous to a global wave that is at the same phase at any latitude and longitude. Figure 4.1 shows an example of gravity wave perturbation on an unperturbed neutral temperature profile obtained from MSIS-E 90 for a specific time, latitude, and longitude. Note that this generation of a gravity wave is very simplistic and does not include all the complex characteristics of a real gravity wave. A true gravity wave would also have associated variations in the winds and densities which we have neglected. These simplifications were used because our focus is on the detection of temperature changes.

![Figure 4.1](image)

**Figure 4.1:** Example of gravity wave perturbations. The orange line is the neutral temperature profile from MSIS-E 90, and the blue line is a 20% perturbation of the profile with a vertical wavelength of 15km.

The OPAL instrument has the 7 imaging slits to have horizontal detection of gravity waves. Equation 4.1 can be modified to also include terms that create a horizontal wave
structure imposed onto the vertical.

\[ T_{\text{wave}}(\text{lat}, \text{lon}, z) = T_N(\text{lat}, \text{lon}, z) \cdot \Delta T[\sin(k_{\text{lat}} \cdot \text{lat}) + \sin(k_{\text{lon}} \cdot \text{lon})] + T_N(\text{lat}, \text{lon}, z) \]

(4.2)

The additions to this equation from Equation 4.1 are the wavenumbers, \( k_{\text{lat}} \) and \( k_{\text{lon}} \), that are defined as \( k_{\text{lat}} = \left( \frac{111}{\lambda_{\text{lat}}} \right) \) and \( k_{\text{lon}} = \left( \frac{111 \cdot \cos(\text{lat})}{\lambda_{\text{lon}}} \right) \). The wave numbers include a factor of 111 and 111\cdot \cos(\text{lat}), which corresponds to the number of kilometers in one degree of latitude and longitude, respectively. Figure 4.2 shows an example of a wave perturbation using Equation 4.2, where the wave is applied to a background temperature of 350K (corresponds to about 110-120km altitude). Also shown in Figure 4.2 are the center LOS of each of OPAL’s seven slits. Clearly seen is a wave structure with max/min of ±20% at wavelength of 300 km.

![Figure 4.2: Model of global horizontal perturbations with a 300km wavelength imposed with the LOS of OPAL’s slits’ view.](image)
4.3 Wave Detection

With the process for wave production in the simulated atmosphere in place, analysis can be performed on single slit and multi-slit signals. This analysis will include an evaluation of OPAL’s minimum wave resolutions including possible interference from sub-resolution waves, and the importance of establishing a background signal. One second integration times are used to preserve the wave signature.

4.3.1 Single Slit Analysis

The horizontal resolution of the OPAL instrument is reported in Chapter 1 as 1 km. Using the Nyquist theorem this can be used to determine the minimum wavelength resolvable by OPAL. This sets the lower limit for the vertical wavelength detection at 4 km, as it must be two times the minimum ‘peak’ to ‘peak’ within two pixels of the CCD.

Figure 4.3(a) shows an example of a one second integration of the virtual CCD image of a single slit with a 4 km vertical wave perturbing the neutral temperature by 20% from the background atmosphere. Figure 4.3(b) is similar to Figure 4.3(a), but this time without the perturbation. Figure 4.3(c) shows the subtraction of the unperturbed signal from the perturbed one and reveals perturbations in the signal in pixel columns that represent altitude perturbations. There is an evident vertical intensity oscillation of approximately 5% of the total signal present in the background image (Figure 4.3(b)), shown in Figure 4.3(d), in pixels with approximately the same wavelength as the vertical wave inputs of the model. A FFT (Fast Fourier Transform) was performed on a single bin’s altitudinal signal in Figure 4.3(e), and reveals a peak near 4 km. The FFT is slightly skewed to the left of the 4-tick mark due possibly to the lack of zero padding from the simulated output which resulted in larger frequency bins, but there are no other signs of an additional wave in the data set. This analysis indicates the capability of OPAL’s measurements to detect gravity wave perturbations in the atmosphere.

To further demonstrate the effectiveness of this analysis on other waves, a perturbation with a 15 km wavelength was tested. The results of this analysis are shown, similarly to Figure 4.3, in Figure 4.4. Shown are (a) the one second integration virtual CCD image of a
single slit, but this time with a 15 km vertical wave perturbing the neutral temperature 20% from the modeled atmosphere is measured; (b) the background image; (c) the residual signal from subtracting the background from the perturbed signal. Clearly seen in Figure 4.4(c), there are perturbations in the signal in pixel columns that represent altitude perturbations. There is an evident harmonic vertical intensity oscillation, shown in Figure 4.4(d), in column 20 of the CCD. A FFT (Fast Fourier Transform) is then done on bin 20’s altitudinal signal which is shown in Figure 4.4(e), and gives a peak representing the 15 km vertical signal perturbation. The results from the FFT exhibit a broader peak than for the 4 km wave, and also shows the same shift to slightly lower wavelengths (the order of a couple kilometer shift as opposed to the fraction of a kilometer shifted in the 4 km analysis).
Figure 4.3: Analysis of 1 second integrated 4 km vertical wave in 1 imaging slit. (a) One second integration of the atmosphere with 4 km vertical wavelength at a 20% perturbation of the neutral temperature. (b) The one second background (unperturbed) image. (c) Result of the integrated wave signal minus the background. (d) Perturbed signal minus background signal of bin 20 plotted as a function of altitudinal pixels to show the harmonic oscillations that an FFT analysis would define. (e) An FFT of bin 20 from (c) to determine oscillations in the vertical signal.
Figure 4.4: Similar to Figure 4.3, but with a superimposed temperature perturbation of 15 km vertical wavelength.
4.3.2 Full Slit Array Analysis

Applying the signal of the full slit array allows for testing the detection of horizontal wave parameters. The horizontal resolution can be applied to the Nyquist theorem to have a resolvable structure of 200 km. For this analysis a similar approach to the single slit analysis in Section 4.3.1 is used by starting with the signal from a perturbed atmosphere. However, the horizontal parameter analysis requires the integrated signal from a single slit to be compared with those from the other slits. Figure 4.5 shows an example of this comparison for a case when no perturbations were introduced. The resulting structure appear from the seven slits to be a wave in the atmosphere, but instead is due to the curvature of the Earth. This is a persistent feature that is, however, eliminated when subtracting the background signal.

Figure 4.6(a), shows in the OPAL signal for each of the seven slits associated with a temperature perturbed by 20% 5 km vertical and 400 km horizontal wavelength.

![Graph showing signal across slits](image)

**Figure 4.5:** Sum of counts on each slits CCD area plotted as a function of their distance from the center slit with a perturbed signal of 5 km vertically and 100 km horizontally.
Similarly the middle panel of Figure 4.6 shows the background signals of the seven slits. Figure 4.6 bottom panel is obtained by subtracting the background of each respective slit from its corresponding perturbed value to reveal the underlying structure. The bottom panel shows the individual slits still exhibit vertical structure in the changes of emission counts, and from slit to slit there is a change in the overall magnitude of the scale that translates into the total counts of the CCD area of each image. The total counts are integrated and shown in Figure 4.7 to present the horizontal structure in emission changes due to the horizontal temperature perturbation imposed in the model.
Figure 4.6: (a) Virtual CCD separated by slit image with 1 second integration of 20% perturbed atmospheric temperature by 15 km vertical and 300 km horizontal wavelength with color bar units of photons per second. (b) Virtual CCD separated by slit image with 1 second integration of background, unperturbed, atmospheric temperature with color bar units of photons per second. (c) Virtual CCD separated by slit image with 1 second integration of 20% perturbed atmospheric temperature by 15 km vertical and 300 km horizontal wavelength with color bar units of photons per second.
Figure 4.7: Sum of counts on each slits CCD area, after subtracting off background emissions, plotted as a function of their distance from the center slit.

4.3.3 Sub-resolution Wave Interference

Attempting to go below the Nyquist frequency, as expected, yields erroneous results, but can be important to understanding the behavior of OPAL when observing of wavelengths below its resolvable range. Figure 4.8(a) is the one second integration of the single slit viewing a 2 km vertical wave perturbing the neutral temperature 20% from the modeled atmosphere. The same process is performed by subtracting the background, unperturbed, atmosphere image (Figure 4.8(b)) to obtain Figure 4.8(c). Figure 4.8(c) visibly has the peak-to-peak features of 2 km but not consistently throughout any of the bins. This inconsistency is reflected in the FFT in Figure 4.8(d) where the main peak is at a 12 km’s frequency. The tail at the low wavelength end shows an nonphysical peak at 12 km. This indicates that small wavelength waves can cause large wavelength artifacts in an FFT analysis of the vertical signal. However, this is an idealized approach and the same process that creates this artifact can wipe it out with real-time integration of the signal, or create an aliasing of the signal to perceive a different wavelength in the FFT analysis. This characteristic is
shown in Figure 4.10, where the 2 km wave matches too closely to the bins and can cause the peaks and troughs to cancel out.

To show the same trends persist with wavelengths below the resolvable distances of OPAL the analysis is redone with a 1 km vertical wave. Figure 4.9(c) already shows perturbations that are clearly not on 1 km wavelength, even though that was the input of the atmospheric model integrated in Figure 4.9(a). The FFT, Figure 4.9(d), confirms that concern with a peak of 6 km from the 1 km input which Figure 4.9(e) corroborates the 6 km oscillation.
Figure 4.8: Analysis of 1 second integrated 2 km vertical wave in 1 imaging slit who’s color bar units are photons per second incident on the CCD. (a) One second integration of the atmosphere with 2 km vertical wavelength at a 20% perturbation of the neutral temperature. (b) The one second background (unperturbed) image. (c) Result of the integrated wave signal minus the background. (d) An FFT of bin 20 from (c) to determine oscillations in the vertical signal. (e) Perturbed signal minus background signal of bin 20 plotted as a function of altitudinal pixels.
Figure 4.9: Analysis of 1 second integrated 1 km vertical wave in 1 imaging slit who’s color bar units are photons per second incident on the CCD. (a) One second integration of the atmosphere with 1 km vertical wavelength at a 20% perturbation of the neutral temperature. (b) The one second background (unperturbed) image. (c) Result of the integrated wave signal minus the background. (d) An FFT of bin 20 from (c) to determine oscillations in the vertical signal. (e) Perturbed signal minus background signal of bin 20 plotted as a function of altitudinal pixels.
Figure 4.10: Diagram of possible aliasing effects due to poor spatial sampling compared to wavelength being observed.

A linear combination of the 2 km and 4 km vertical waves are introduced to the atmospheric model, with the same 20% temperature disturbance, to confirm whether the small wavelength artifact remains or is dominated by the resolvable wavelength’s signal. Now the combined waves’ 1 second integrated image, Figure 4.11(a), is subtracted from the background image, Figure 4.11(b), to produce another plot with the signal perturbations shown in Figure 4.11(c). By observation, the signal perturbation is much more difficult to see the wavelengths involved with this resulting image. However, the FFT in Figure 4.8(d) is able to resolve a sharper peak at 4 km than that centered at the erroneous artifact of the sub-resolution wave at 12 km.
4.4 Averaged Background

The analysis so far presented required the knowledge of the unperturbed background signals. In reality this background is needs to be estimated. Investigating the use of an averaged background that is built from a series of OPAL observations is a necessary step in advancing the analysis for OPAL’s gravity wave analysis. Figure 4.12(b) shows an average of the signals from five individual CCD images that were generated using imposed perturbations of 5 km, 10 km, 15 km, 20 km, and 25 km vertical wavelengths. Next the averaged background is used to analyze a different wave perturbation (4 km vertical wavelength) which is shown Figure 4.12(c). Following the analysis used for the other single slit structures, Section 4.3.1, bin 20’s signal was analyzed. Figure 4.12(e) shows that the vertical oscillations are not as smooth as seen in the previous analysis of the 4 km vertical wave (Figure 4.3(d)). However, the FFT in Figure 4.12(d) is still able to resolve the 4 km structure of the pixel column (consistent with the slight shift to longer wavelengths). There are also large wavelength artifacts weighing the FFT to the right. Overall, this analysis shows that using an average background is a viable method for OPAL to determine wave characteristics from its own data.
Figure 4.11: Analysis of 1 second integrated 2 km and 4 km vertical wave in 1 imaging slit with color bar units of photons per second incident on the CCD. (a) One second integration of the atmosphere with 2 km and 4 km vertical wavelength at a 20% perturbation of the neutral temperature. (b) The one second background (unperturbed) image. (c) Result of the integrated wave signal minus the background. (d) An FFT of bin 20 from (c) to determine oscillations in the vertical signal. (e) Perturbed signal minus background signal of bin 20 plotted as a function of altitudinal pixels.
Figure 4.12: Analysis of 1 second integrated 4 km vertical wave by subtracting an average-made background CCD image. (a) 1 imaging slit with color bar units of photons per second incident on the CCD using an averaged background (b) to determine detect ability using other wave data. (c) Result of the integrated wave signal minus the background. (d) An FFT of bin 20 from (c) to determine oscillations in the vertical signal. (e) Perturbed signal minus background signal of bin 20.
4.5 Signal to Noise Analysis

I order to check the wave analysis’ ability to detect gravity wave perturbations, the signal to noise (SNR) of the instrument needs to be understood. The inverse of the SNR is the uncertainty associated with a measurement, and the perturbation in the signal seen in the single and multiple slit analysis was shown to be $\sim 5\%$. Therefore, to determine whether the wave perturbations in the signal can be confidently determined the SNR must be greater than 20 to have an uncertainty in the CCD image be less than the perturbation of the signal.

A radiometric analysis of the OPAL detector is done to calculate the SNR as a function of integration time ($t_{int}$). There are three sources of noise that are considered for this CCD: the photon noise (PN-also known as shot noise), dark noise (DN), and the read noise (RN). They are combined by the sum of their squares to give the SNR as,

$$SNR = \frac{Signal \cdot t_{int}}{\sqrt{PN^2 + DN^2 + RN^2}}$$  \hspace{1cm} (4.3)

Photon noise is defined as, $PN = \sqrt{Signal \cdot t_{int}}$. The CCD characteristics given in Table 1.1 define the read noise and dark noise. Read noise $RN = (readout noise) \cdot (readout rate) \cdot t_{int}$. The dark noise is the weakest noise considered as the estimated temperature of OPAL in its low Earth orbit is 10°C and results in only 0.1 electrons per second as dark current. Therefore the dark noise is shown to be, $DN = 0.1 \cdot t_{int}$ [Palmer and Grant, 2010]. The signal from the 1 second integrated background from the OPAL position described in Table 3.1, mid-latitude region, from MSIS-E 90 data (at 13.5 UT 2015 day of year 13.5 with a moderate F10.7a of 130) is used in the SNR Equation 4.3 to produce Figure 4.13. This figure shows the SNR increases, as expected, with the lengthening of the integration time, and the SNR at higher altitudes is decreases from lower altitudes due to smaller volume emission rates in that region. There are large regions of integration and altitude ranges with SNR above 20, however, the smallest integration possible is needed to observe the spatially and temporally restricted gravity wave in the OPAL FOV. Figure 4.5 shows the SNR as a function of altitude for both a 1 second, Figure 4.14(a), and 5 seconds,
Figure 4.14(b). The 1 second integration has some of the lower altitudes, below $\sim 87$ km, with SNR greater than 20. And the 5 second integration shows the region of 20 SNR goes to an altitude of $\sim 105$ km. The 5 second integration will result in a larger altitude for sampling the wavelengths present in the signal, but the 5 seconds means that OPAL is moving $\sim 35$ km and would also smear the signal of the waves.

This SNR analysis is confirmed by the work previously done by Marchant et al. 2014, who reported on predicted range in SNR values of 40 at the top and 400 at the bottom of the limb using an integration time of 20 seconds. Figure 4.15 shows the modeled SNR has values at the lower and higher tangent altitudes of this analysis’ values at the 20 second integration time. A reason for the disparity of the higher altitude SNR with Marchant et al. 2014 is the original launch was expected in the solar maximum (2014) and would have greater emission with more solar activity at those altitudes, while this current model is run expecting the current solar minimum. Therefore, the change from 40 SNR, shown by Marchant et al. 2014, to 14, in Figure 4.15 can be expected.

Figure 4.13: The log color plot of signal to noise ratio shown as functions of altitude and integration time. There are also contour lines that give constant signal to noise at 10, 20, and 100, which represent regions of 10%, 5%, and 1% uncertainty respectively.
Figure 4.14: SNR analysis of 1 sec and 5 sec integration. The blue line is the SNR as a function of altitude, and the orange line marks the SNR of 20 for each integration time.

Figure 4.15: A logplot of SNR shows the agreement of values previously derives from Marchant et al. 2014.
5.1 Conclusion

The primary purpose of this research is to develop a model of the OPAL instrument’s CCD detector to determine the resolution and detect ability of atmospheric gravity waves in the lower thermosphere from $O_2$ A-band emissions. Understanding of the $O_2$ A-band and how it is integrated into OPAL’s output is needed to achieve this goal.

Modeling the OPAL observation requires the volume emission rate (VER) to be calculated at each point along the integrated line of sight (LOS). The atmospheric processes that produce the A-band emission as an input to the VER is producible at any latitude, longitude, or altitude in the range of OPAL’s field of view (FOV). The temperature dependent spectrum of the $O_2$ A-band is carried through the integration and weighted with the VER. Furthermore, the OPAL cubsat’s orbital mechanics are modeled to provide line of sight (LOS) for the emissions to integrate over. Thus, resulting in a virtual CCD image of the OPAL output. This synthetic OPAL observation is analyzed to determine resolveability of gravity waves in the OPAL output with care to determine the lower threshold of wavelength that can be detected by the instrument.

This work will provide incentive for OPAL to have a gravity wave campaign mode with shorter integration times over gravity wave ‘hot spots’ that can detect the smaller spectrum of gravity waves seen propagating in the lower thermosphere. A precise integration time cannot be specified at this time. Calculating the needed integration time depends on specifications of the OPAL instrument’s integrated noise that has not been calibrated yet. The noise experienced by the detector will put an upper limit on the wavelengths able to be detected by OPAL as the higher altitude signal will be over taken by the noise for lower integration times.
5.2 Future Work

Much has been learned from the OPAL gravity wave analysis of detailed insights into the expectations of resolveability and detectability of the OPAL instrument in flight. The model can be further improved for better analysis of the wave detection, and in efforts of the effects of solar activity on the temperature profile.

The wave analysis done in this thesis utilized sanitized wave structures implemented in this model. Further work could be done applying more realistic waves to result in analysis closer to the real OPAL data. This would include waves with varying perturbation strengths of the temperature, spatially limiting the waves, and changing orientation of the horizontal waves. All of these would greatly enhance understanding of gravity wave observations with the OPAL cubesatellite.

To achieve the science goal of understanding solar storm’s effects on the thermospheric temperature, there needs to be a conversion from the OPAL output to temperature. This is achievable with the information of temperature dependent line strengths discussed in Chapter 2. The virtual CCD provides the line strengths at each tangent altitude’s line of sight signal. However, this technique would only be appropriate if the majority of signal comes from the tangent altitude. The Figure 5.2 shows that this is not the case, with the ratio of signal from within 1 km of the tangent point to the total integrated signal at each altitude. It is evident within the plot that a majority of the signal does not come from the lowest 1 km with the highest peak of the ratio at 40%. This suggest an inversion method is beneficial to produce a more accurate temperature profile from the OPAL signal prior to fitting the line strengths to their temperature dependence.
Figure 5.1: Plot of the ratio of signal coming from the lowest 1 km of the line of sight (LOS).
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