UV AND VISIBLE RADIATION FROM MAGNESIUM POWDER COMBUSTION IN AIR

A Thesis in
Aerospace Engineering
by
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ABSTRACT

Dense cloud powdered magnesium jet deflagration was studied using a linear test combustor. Magnesium is a highly flammable metal that produces copious ultraviolet and visible light emissions during combustion. Understanding of the radiant emission and combustion temperatures is important for application to power and propulsion. Because of the large amounts of broadband UV available and the fact that magnesium emits strongly at germicidal wavelengths indicates a possible anti-bacterial application as well. Two calibration lamps with known values of spectral irradiance and color temperature were used to validate UV and visible wavelength flux measurement and temperature measurement techniques. Silicon photo-diode detectors sensitive to UV were used to determine broadband flux. Collimators, a CCD camera and spectroscope were used to measure spectral emissions in the UV and visible spectrums. Comparison of spectral emissions was compared to Planck’s law predictions using an automated algorithm to permit inference of combustion temperatures. Comparison with the temperature standard indicated an error of ~ 60 K at 3000 K temperature. Spectral extinction coefficients in a bacteria suspension were also measured as a function of concentration. These procedures were applied to measurements in a linear magnesium powder and air combustor. The flame temperature of magnesium combustion was determined to range from 2500-3500 K, depending on the location and air/fuel ratio. The predicted temperatures are comparable to previously published data and to values found from adiabatic flame temperature predictions using a chemical equilibrium computer code. The broadband UV fluxes emitted at different locations were also measured.
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NOMENCLATURE

a Efffective particle radius
a_i Activity
a_n Mie scattering coefficient
A_{ij} Coefficient on
A_n Coefficients related to Mie scattering coefficients
b_i Number of moles of j
b_n Mie scattering coefficient
c_o Speed of light
C_{abs} Absorption cross section
C_{ext} Extinction cross section
C_p Specific heat
C_{sca} Scattering cross section
E Cloud hemispherical emissivity
E_{bb}λ Black-body emissive power
E_w Emissivity of the wall
G_i Total free energy
ΔG_i Standard free energy
h Planck’s constant
h_n Spherical Bessel function of 3rd kind
ΔH_i Enthalpy
ΔH_{f}^* Standard free energy of formation
H_{n+1/2} Bessel function of 3rd kind
I_{1,2} Nondimensional polarized intensities
I Transmitted intensity
I_{in} Incident unpolarized beam strength
I_o Incident intensity
I_{sca} Intensity of scattered radiation
I_{1} Intensity
J_{n} Spherical Bessel function of 1st kind
J Irradiance
J_{n+1/2} Bessel function of 1st kind
K_a Absorption Optical Coefficient
K_s Scattering Optical Coefficient
k Boltzmann’s constant
m index of refraction
Mg Magnesium
MgO Magnesium Oxide
N Air/fuel ratio
n_i Molar amount
N Total number of moles
N_2 Nitrogen
N T Number of particles
O_{2} Oxygen
P Pressure
P_n Legendre polynomials
Q Heat released/Emitted flux
Q Gain Radiative flux
Q_{abs} Absorption efficiency factor
Q_{ext} Extinction efficiency factor
Q_{sca} Scattering efficiency factor
r_p Particle radius
R Gas constant
R_w Radius to wall
R_{ab} Spectral radiance
s Path length
δ Unit vector
S_{1,2} Complex amplitude functions
S_{i} Absolute entropy
ΔS_i Entropy
T Temperature
T P Particle temperature
T_w Temperature of wall
x Size parameter
X_i Number of moles of reactant
Y_i Number of moles of product
z Nondimensional spectral variable
α Absorptance
β_λ Extinction coefficient
ε Effective emissivity
ε Emittance
ζ_n Riccati-Bessel function
Θ Scattering angle
κ_λ Absorption coefficient
λ Wavelength
π_{nx} τ_n Direction dependent functions
ρ Reflectance
ρ_m Mixture density
σ Stefan-Boltzmann constant
σ_λ Scattering coefficient
τ Transmittance or transmissivity
τ L Optical thickness
ϕ Scattering phase function
ψ_n Riccati-Bessel function
Ω Solid Angle
ω Albedo
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Chapter 1: Introduction

1.1 Background and Motivation

Magnesium is a highly reactive metal and is easily ignited while in powdered form. For this reason magnesium has been used as a fuel component in solid propellants, pyrolants, and pyrotechnics. For use in solid propellants, Singh et al. [1] and Singh and Rao [2] have described grains that are superstoichiometrically loaded with magnesium for ramjet propulsion applications. Shafirovich et al. [3] and Miller and White [4] have both described the use of magnesium powders for extra-terrestrial and underwater thruster applications. Pyrolants often use superstoichiometric metal loads to produce large amounts of molten metal for ignition of larger conventional solid propellant grains. Discussion of both Teflon-Mg and NaNO₃ –Mg systems are described elsewhere [5, 6]. Use of magnesium combustion in fireworks is common [7, 8] and can be traced to 1865 [9], and its use in photographic flash powder to the earliest days of photography [10]. One of the hallmarks of magnesium combustion is the emission of copious amounts of thermal and electro-magnetic radiation. The high temperatures of these combustion processes push the emission spectrum of the radiation into the visible, near-UV, and UV ranges. Here UVA, UVB, UVC, and visible ranges are defined as 0.315-0.4, 0.28-0.315, 0.1-0.28, and 0.4-0.7 μm, respectively.

In addition to broadband ultraviolet (UV) emission, the combustion of magnesium also produces UV emission in peaks at specific wavelengths (of special interest is the 0.285 μm line). These correspond to the wavelengths used in germicidal lamps for sterilization purposes. Microorganisms, such as, vegetative pathogens, spores, and biotoxins are relatively easy to kill with UV radiation [11]. UV light can rapidly kill spores in either of two ways. It can mutate the nucleic acids in the DNA, which prevents reproduction, or it can damage the protein on the outer surface of the spore so that the vegetative cell does not function. Damaging biotoxins or killing spores and viruses quickly requires very strong UV radiation in
the 260 and 285 nm bands. Magnesium will emit radiation around these wavelength ranges.

Furthermore, broadband UV radiation levels of $10^4 \mu \text{W-sec/cm}^2$ will kill virtually all known pathogens, given sufficient time, according to standard germicidal UV water purification tables [12]. The reaction also produces high thermal radiation that can produce incineration of a biological agent. Magnesium also has a controllable burn rate, and completely safe fallout, since magnesium oxide is benign.

Because of these reasons, a study of the UV and visible light radiation emitted by magnesium and air deflagration was undertaken. These experiments utilized a linear metal powder combustor. Very high fluxes are available from using the linear combustor. The purpose of this thesis is to describe the experimental test apparatus used to measure the UV emission from burning Mg clouds, the theoretical basis of these emissions, the temperatures that produce the emissions, and the extinction coefficients of the bacterial solutions exposed to those emissions.

### 1.2 Metal Combustion

Research involving the combustion of metal particle fuels at the Applied Research Lab (ARL)/Penn State has been an ongoing topic for over a decade. Most of the work has focused on aluminum or aluminum-based fuels with a range of particle sizes (see Moore et al. [13] and Miller [14]).

Dreizin et al. [15] burned free-falling individual magnesium particles in air. They monitored the particle combustion temperatures and compared black-body and MgO radiation histories. They also observed that the intensity of the radiation bands of Mg and MgO vapors were significant after particle ignition but became indistinguishable from the black-body radiation at later combustion times. Therefore they proposed that oxygen diffuses to the surface of the burning particles and is dissolved in
liquid magnesium. They suggested a new phase in which liquid MgO is formed inside the burning Mg particles.

The combustion spectra of loose Mg particles in air and carbon dioxide at atmospheric pressure were investigated by Valov et al. [16]. They plotted combustion time as a function of initial particle size and observed that the magnesium oxide vapor disappears before the vapor of the metal itself when combustion takes place in carbon dioxide. They concluded that this was because of the gas-phase reaction.

In any combustion reaction a fuel reacts with an oxidizer; in air, this is usually oxygen, although CO₂ and water vapor may react as well. The basic magnesium combustion reaction is shown as,

\[2Mg + O_2 \rightarrow 2MgO + heat\] (1.1)

where the magnesium element is the fuel. In this reaction the metal is converted to a metal oxide and heat and light are generated. From a basic calculation of the amount of heat released, magnesium was found to have a lower heating value of roughly 23,000 KJ/kg. The combustion of magnesium and other metal particles in air is characterized by high flame temperatures, bright visible flames, and emission of broad and narrow band UV. When a material is heated it gives off thermal radiation, the higher the temperature the greater the magnitude of emitted radiation, and the more strongly skewed that radiation is to shorter wavelength or higher frequency emission.

Figure 1.1 illustrates schematically the main features of magnesium droplet combustion. In common with hydrocarbon combustion, magnesium combustion is generally characterized by vapor phase combustion, in which magnesium evaporates from the molten droplet surface. Magnesium vapor reacts with the oxidizer diffusing into the combustion zone from the surrounding atmosphere. The reaction zone occurs in the volume surrounding the metal particle at a distance to particle dictated by
metal evaporation rate outwards and gas diffusion rate inwards. This displacement is a function of temperature, pressure, and the degree of atmospheric vitiation (see Miller and Garza [17]).

A kinetics based model for this process has been presented by Miller and Garza [17]. This model shows that in agreement with Rosner’s ideas [18], a vapor phase combustion process can be monitored so long as the rate of evaporation is sufficient to overcome the influx of oxidizer. It is not necessary for the droplet surface to equal the magnesium saturation temperature for a given pressure. However, if the droplet surface temperature is too low, then the reaction can be pushed to the surface of the droplet. The surface reaction is substantially smaller than the vapor phase reaction rate. For small particles, chemical kinetic reactions are the primary mechanisms. For larger droplets (roughly those larger than one micron) the kinetic reaction rate is very fast relative to the rate of diffusion of oxidizer though the gaseous product layer to the evaporated fuel. The MgO oxide products either recondense or freeze on the droplet (~20%) or form submicron sized smoke (~80%).

For particles of interest here, the droplet burn time should correlate with approximately the square of the initial droplet diameter, due to the reaction being primarily diffusion dominated [17]. The reaction behavior strongly impacts the size of the metal oxide particles produced and therefore should impact the effectiveness of the oxide as an anti-microbial agent. The combined effect of the reaction rate and the Mg or MgO droplet size (i.e. the area available for thermal radiation emissions) has a strong impact on the radiated flux produced.
When a combustion process takes place adiabatically (with no heat loss or gain), the temperature of the products is referred to as the adiabatic flame temperature. It is a function of the heat of formation and enthalpies of the reactants and those of the reaction products. Product dissociation has an impact by taking up some of the reaction energy to breakup molecules.

Magnesium’s flame temperature has been measured anywhere from 2000K to 3000K [19-21], in many instances depending on the oxidizer type and its temperature or pressure. Shoshin and Dreizen [19] report 3000 +/- 200 K in burning aerosols. Florko and coworkers have described a range: 2630 K [20], 2900 K [21], and 3000 K [22]. The lower temperature measurements correspond to single particles, while the larger measurements were made of reacting aerosols. In common with many metal
combustion systems, phase change processes play a very strong role defining temperatures in the reaction processes. These processes include dissociation temperature of the oxide, oxide melting point, metal melting point, and latent heat of phase transformation. For example aluminum combustion temperatures are typically limited by the temperature at which the dissociation rate of alumina takes off (a strong function of pressure). For magnesium systems, however, the reaction product temperature is usually limited by the large latent heat of melting of MgO, and consequently the theoretical reaction temperature is often the melting point of magnesium oxide, MgO, near 3,100 K, which is not a function of pressure.

Interestingly, the color temperature (that is measured by a thermal pyrometer) is often above 3,900 K [23]. The color temperature of a light source is a characteristic of visible light and is the temperature of an ideal black-body radiator that radiates light of comparable hue to that light source. Newman and Payne [23] saw from their investigation into the combustion of bulk or powdered magnesium or magnesium alloy in air that it burns with a very bright blue-white flame at a very high local temperature. Their quantitative measurement of the color temperature was 3900 K, whereas their thermodynamic calculations showed the adiabatic flame temperature limit as 3100K. They concluded that the color temperature cannot correspond to a real flame temperature because of nonequilibrium effects. As will be discussed later, this had important implications for measurement methods.

Figure 1.2 summarizes the dependence of Mg boiling temperature, and MgO melting, boiling, decomposition, and sublimation temperatures on pressure. The close comparison of reacting magnesium surface temperature (Derevyaga [24]) and the magnesium boiling point curve (Roberts et al. [25]) suggests that the reaction is occurring in the vapor phase. Gol’dshleger and Amosov [26] describe the modes of magnesium combustion for different particle temperatures and oxygen concentration. Below a temperature of 1300 K or at a lower oxygen concentration than 20%, an oscillatory behavior
was observed as it transitioned between surface and gas phase mechanisms. Figure 1.2 also shows sublimation, evaporation, and other data [27-30].

![Figure 1.2: Magnesium and Magnesium Oxide Phase Change Temperature Dependence on Pressure [24-30]](image)

It is significant to note that thermal radiation acts to reduce the reaction product temperatures of a single particle by redistributing energy to other locations. In a reacting aerosol the redistributed energy goes to other particles of the combustion cloud so the temperature impact is less. The degree of reduction is impacted by the concentration or optical thickness of the cloud, due to the fact that at some point the fuel cloud starts to use up all the oxidizer in the surrounding gas. Also reaction in a dense particle cloud (as opposed to a single particle or droplet) produces a different burn rate.
The air-fuel ratio is the mass ratio of air to fuel present during combustion. When the fuel is combined with all the free oxygen and is chemically balanced it is referred to a stoichiometric mixture. For Mg and air combustion any mixture with an air-fuel ratio of less than 0.62 is considered to be a rich mixture, whereas any more than 0.62 is a lean mixture. If dissociation effects are neglected, then the stoichiometric air/fuel ratio should produce the maximum adiabatic flame temperature. This is because the excess fuel in a rich mixture and excess oxygen in a lean mixture takes energy that would otherwise go towards heating the products of combustion. In a particle/oxidizer cloud, even though the initial composition is near stoichiometric, as the reaction proceeds and more product vapors accrue and oxygen is depleted, the reaction rate and temperatures will be reduced.
Chapter 2: Theory

2.1 Black-body and Gray Body Radiation

When thermal radiation impinges on an object of finite thickness, there are three outcomes; some of the radiation will be reflected away from the surface, a fraction will be absorbed by the material and the rest will be transmitted through the slab. Figure 2.1 shows a sketch of this process, where the gray section represents a slab.

![Figure 2.1: Reflection, Absorption, and Transmission by a Slab](image)

The three radiative properties derived from these outcomes are defined as follows,

\[
\rho = \frac{\text{reflected part of incoming radiation}}{\text{total incoming radiation}} \quad (2.1)
\]

\[
\alpha = \frac{\text{absorbed part of incoming radiation}}{\text{total incoming radiation}} \quad (2.2)
\]
Since the incoming radiation must be absorbed, reflected, or transmitted, the following must be true,

\[ \alpha + \rho + \tau = 1 \]  \hspace{1cm} (2.4)

Obviously these nondimensional properties have a magnitude between 0 and 1.

A fourth nondimensional property of emittance can be defined since all surfaces also emit thermal radiation.

\[ \varepsilon = \frac{\text{energy emitted from a surface}}{\text{energy emitted by a blackbody surface at same temperature}} \]  \hspace{1cm} (2.5)

The emissivity is a property of a material that describes its ability to emit energy by radiation. This is the ratio of energy radiated by the material to energy radiated by a black-body at the same temperature. It is essentially a measure of a material’s ability to radiate absorbed energy.

A black-body is an idealized object that absorbs all electromagnetic radiation. There is no radiation that passes through a black-body or that is reflected from the surface of the object. A black-body has an emissivity equal to 1. Since no material existing in nature behaves precisely as a black-body, another more useful approximation referred to as gray bodies are used. Gray surfaces do not absorb or emit the full amount of radiative flux. They instead radiate a portion of the black-body radiation, which is characterized by the object’s total constant emissivity, which is assumed constant over all wavelengths.

Planck’s law of black-body radiation describes the spectral radiance of electromagnetic radiation. The black-body emissive power distribution or Planck’s law is,
where λ is the wavelength, n is a constant refractive index, k is Boltzmann’s constant, c₀ is the speed of light, and h is Planck’s constant. The following constants can be defined in order to simplify equation 2.6

\[ C_1 = 2\pi hc_0^2 = 3.7418 \times 10^{-16} \text{ Wm}^2 \] (2.7)

\[ C_2 = \frac{hc_0}{k} = 14,388 \mu mK = 1.4388 \text{ cmK} . \] (2.8)

The “-1” in the brackets of the denominator can be neglected for large values of

\[ \exp \left( \frac{hc_0}{n\lambda kT} \right) , \] leading to Wien’s law. The black-body emissive power, E_{b\lambda}, can be written per unit frequency or wavelength. Planck’s law of black-body radiation for several different temperatures is plotted in Figure 2.2 Germicidal lamps operate at a wavelength of 253.8 nm in the UV spectrum. With magnesium combustion happening at a temperature of about 3050 K, a power output of roughly 2000 W/m² can be expected. Figure 2.2 illustrates the magnitude of black-body emissive power as a function of wavelength and emitting body temperature.
Wien’s displacement law relates the spectrum of black-body radiation at any temperature to the spectrum at any other temperature,

\[ \lambda_{\text{max}} T = C_3 = 2898 \text{ } \mu\text{m} \text{ } \text{K} \tag{2.9} \]

It shows that the wavelength at which the intensity of the radiation is a maximum is a function of only temperature. Thermal pyrometry takes advantage of this, but requires a good estimate of gray body emissivity. The Stefan-Boltzmann law describes the total energy radiated per unit surface area in time (also known as the irradiance, radiant flux, or emissive power). This equation for a gray body as a function of temperature is,
\[ J = \varepsilon \sigma T^4 \] (2.10)

where the Stefan-Boltzmann constant, \( \sigma \), equals \( 5.67 \times 10^{-8} \) \( W/\text{m}^2\text{K}^4 \), \( J \) is the irradiance, and \( \varepsilon \) here is the gray body emissivity. The fractional amount of gray body flux in a given wavelength range can be estimated by,

\[
f(n\lambda T) = \frac{\int_{\lambda_1}^{\lambda_2} E_{\lambda}(T, \lambda) d\lambda}{\int_{0}^{\infty} E_{\lambda}(T, \lambda) d\lambda} = \frac{15}{\pi^3} \frac{\xi^3 d\xi}{\int_{C_2/n\lambda T} e^\xi - 1}.
\] (2.11)

where \( C_2 =14,388 \) \( \mu\text{m-K} \).

Two important features of Figure 2.2 deserve discussion. First as temperature increases, the amount of flux of all frequencies (including UV and visible) increase dramatically because of the \( T^4 \) dependence. Second the fraction of total flux that is in the UV and visible ranges also increases dramatically.

### 2.2 Mie Theory

One general theory describing radiative scattering by absorbing spheres is referred to as “Mie Theory”. How the interaction between particles and electromagnetic waves is described is determined by the relative size of the particles compared to the wavelength of radiation. A dimensionless size parameter \( x \) is determined from,

\[
x = \frac{2\pi a}{\lambda}
\] (2.12)

where \( a \) is the effective radius of the particle. This parameter is defined to determine the type of scattering that is present. When \( x << 1 \), Rayleigh scattering is used to describe the nature of this
interact. If $x \gg 1$, the particle can be treated as a normal surface and geometric optics is used to determine the corresponding properties. Mie scattering must be applied when the size of the spherical particle is too large to consider Rayleigh theory, but too small to employ geometric optics, which occurs for $x \sim 1$. This yields over the range of the UV spectrum that the effective radius must be between 72 nm and 130 nm and over the visible range an effective diameter of 200-1200 nm for Mie scattering to be valid. This is an appropriate size for the produced MgO smoke, and may be of significance for the present study, given that \( \sim 80\% \) of MgO product formed is in the form of smoke. Florko and Golovko [20] provide theoretical and empirical arguments that MgO with a characteristic size of 180 nm (0.18 \( \mu \text{m} \)) is the principal emitter in a magnesium/air flame.

The amount of scattering and absorption by a particle can be expressed in terms of efficiency factors, which are nondimensionalized with the projected surface area of the sphere,

\[
Q_{\text{abs}} = \frac{c_{\text{abs}}}{\pi a^2} \hspace{1cm} (2.13)
\]

\[
Q_{\text{sca}} = \frac{c_{\text{sca}}}{\pi a^2} \hspace{1cm} (2.14)
\]

\[
Q_{\text{ext}} = \frac{c_{\text{ext}}}{\pi a^2} \hspace{1cm} (2.15)
\]

where the $c_i$ are the radiation cross-sections. The following expression can be used to related the three efficiency factors,

\[
Q_{\text{ext}} = Q_{\text{abs}} + Q_{\text{sca}}. \hspace{1cm} (2.16)
\]

Through manipulation of these equations shown by Modest [31, 32], the efficiency factors simplify to,
\[
Q_{sca} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n + 1)(|a_n|^2 + |b_n|^2) \tag{2.17}
\]

\[
Q_{ext} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n + 1)\Re(a_n+b_n) \tag{2.18}
\]

where \(a_n\) and \(b_n\) are the Mie scattering coefficients, which are complex functions of \(x\) and \(y = mx\). The extinction efficiency factor is a function of the real part of addition of these scattering coefficients. The Mie scattering coefficients are calculated using the Riccati-Bessel functions, \(\psi_n\) and \(\zeta_n\), as follows.

\[
a_n = \frac{\psi'_n(y)\psi_n(x) - m\psi_n(y)\psi'_n(x)}{\psi'_n(y)\zeta_n(x) - m\psi_n(y)\zeta'_n(x)} \tag{2.19}
\]

\[
b_n = \frac{m\psi'_n(y)\psi_n(x) - \psi_n(y)\psi'_n(x)}{m\psi'_n(y)\zeta_n(x) - \psi_n(y)\zeta'_n(x)} \tag{2.20}
\]

Here \(m\) is the complex index of refraction, \(n\) is a positive integer, and the prime denotes differentiation.

The Riccati-Bessel functions are related to the Bessel and Hankel functions by,

\[
\psi_n(z) = z j_n(z) = \left(\frac{\pi z}{2}\right)^{\frac{1}{2}} J_{n+1/2}(z) \tag{2.21}
\]

\[
\zeta_n(z) = z h_n(z) = \left(\frac{\pi z}{2}\right)^{\frac{1}{2}} H_{n+1/2}(z) \tag{2.22}
\]

where \(J_{n+1/2}\) and \(H_{n+1/2}\) are the Bessel functions of the first and third kind and \(j_n\) and \(h_n\) are the corresponding spherical Bessel functions.

To apply Mie theory, the complex index of refraction must be known. Several studies into these values and the efficiency factors have been completed. Machorro, Siqueriros, and Wang [33] presented values for the optical properties of a magnesium thin film obtained from ellipsometric and absolute reflectance measurements for the infrared and visible spectrum. Hunter [34] measured the index of
refraction of Al and Mg as a function of wavelength. Both authors used a Drude model and found it to be good approximation. Hunter also calculated the extinction coefficient values for Mg of wavelengths 10-120 nm and found the values to range between 0.0005 and 0.4. Plass [35, 36] has studied the Mie scattering of aluminum oxide and magnesium oxide, whereas Florko et al. [37] and Malitson and Stephens [38] determined the absorption efficiency factors of MgO particles for different wavelengths and temperatures.

This work is summarized in Figure 2.3 and shows both the refractive index and extinction coefficient.
Plass [36] determined theoretically the complex index for aluminum oxide and magnesium oxide where,

$$m = n_1 + in_2.$$  \hfill (2.23)

These values are found in Table 1. It was difficult to find indices in the UV, therefore the curves produced from Table 1 were extrapolated. Stephens and Malitson [38] report $n_1 = 1.76$ for a wavelength of 0.4 $\mu$m and nothing for $n_2$.

<table>
<thead>
<tr>
<th>Wavelength</th>
<th>Aluminum oxide</th>
<th>Magnesium oxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0.5 \mu$m</td>
<td>1.77, $10^{-6}$</td>
<td>1.725, $5(10)^{-6}$</td>
</tr>
<tr>
<td>1</td>
<td>1.75, $10^{-6}$</td>
<td>1.720, $7(10)^{-6}$</td>
</tr>
<tr>
<td>2</td>
<td>1.74, $10^{-6}$</td>
<td>1.705, $1.2(10)^{-5}$</td>
</tr>
<tr>
<td>3</td>
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<td>1.690, $1.6(10)^{-5}$</td>
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<td>4</td>
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</tr>
<tr>
<td>5</td>
<td>1.63, $10^{-4}$</td>
<td>1.64, $5(10)^{-5}$</td>
</tr>
<tr>
<td>6</td>
<td>1.54, $2.2(10)^{-4}$</td>
<td>1.60, $10^{-4}$</td>
</tr>
<tr>
<td>8</td>
<td>1.35, $3.3(10)^{-4}$</td>
<td>1.51, $8(10)^{-4}$</td>
</tr>
<tr>
<td>10</td>
<td>1.09, $5(10)^{-4}$</td>
<td>1.44, $9(10)^{-4}$</td>
</tr>
</tbody>
</table>

The extinction and absorption efficiency factors, $Q_{\text{ext}}$ and $Q_{\text{abs}}$, were calculated for magnesium and magnesium oxide particles of varying radii. Figures 2.4-2.5 show predictions of the extinction and absorption efficiencies of Mg particles of 0.2 and 2 $\mu$m diameters. Figures 2.6-2.8 show the same for MgO particles with diameters of 0.2, 2.0, and 20 $\mu$m, and compare them with the predictions of Plass [36]. The agreement is quite good which gives confidence in the theoretical implementation. Figure 2.6 also compares predictions with measurements made for these quantities by Florko et al. [20, 37]. The
predictions for extinction efficiency are in excellent agreement. The predictions of absorption efficiency are orders of magnitude different. This large difference has also been addressed by Florko et al. [37] who attribute it to the use of complex index of refraction coefficients that are measured at lower (25-1000 °C) temperatures than combustion temperatures (~3000 K).

Florko et al. [20] take into account temperature in an expression for $Q_{abs}$ at 0.7 μm:

$$Q_{abs}\mid_{0.7\mu m} = 12 \exp \left( \frac{-19,140K}{T} \right).$$

(2.24)

The modified curve for $Q_{abs}$ in Figure 2.6 was determined from the multiplication of $Q_{abs}$, which was found using methods described earlier, by the ratio of $Q_{abs}$ obtained from using Equation 2.24 to that for 0.7 μm. This curve shows good agreement with measured values.

![Figure 2.4: Extinction and Absorption Efficiency Factors for 0.1 μm Radius Mg Particle](image)
Figure 2.5: Extinction and Absorption Efficiency Factors for 1 μm Radius Mg Particle

Figure 2.6: Extinction and Absorption Efficiency Factors for 0.1 μm Radius MgO Particle
Figure 2.7: Extinction and Absorption Efficiency Factors for 1μm Radius MgO Particle

Figure 2.8: Extinction and Absorption Efficiency Factors for 10μm Radius MgO Particle
Plass [36] suggests that the effective emissivity of particles can be expressed by:

\[ \varepsilon = C \frac{Q_{abs}}{\sqrt{Q_{sca}}} \]  

(2.25)

Here the constant C is an approximate value of 2.3. This equation is valid when the absorption cross section is very much less than the scattering cross section and yields the maximum emissivity possible for a very large number of particles. Comparisons of the emissivity prediction made using this expression and measurements of Florko et al. [21] and Florko and Golovko [20] are shown in Figure 2.9. This shows excellent agreement for wavelengths greater than 600 nm, and for smaller MgO particles.

Figure 2.9: Emissivity of MgO
2.3 Radiative Properties

2.3.1 Radiative Properties of a Particle Cloud

The fraction of energy scattered by all particles per unit length along the direction of the incident beam is referred to as the scattering coefficient. It equals the scattering cross-section summed over all particles. For a cloud of uniform size particles of radius $a$, the scattering, absorption and extinction coefficients are respectively,

$$
\sigma_{s\lambda} = N_T C_{sca} = \pi a^2 N_T Q_{sca}
$$

(2.26)

$$
\kappa_{\lambda} = N_T C_{abs} = \pi a^2 N_T Q_{abs}
$$

(2.27)

$$
\beta_{\lambda} = \kappa_{\lambda} + \sigma_{s\lambda} = N_T C_{ext} = \pi a^2 N_T Q_{ext}
$$

(2.28)

where $N_T$ is the number of particles per unit volume.

2.3.2 Attenuation by Absorption and Scattering

Attenuation, or extinction, is the gradual loss in intensity of any kind of flux through a medium. In a solid-liquid suspension, both the solids and the liquid absorb and scatter part of the radiant causing attenuation. The attenuation caused by scattering, or “out-scattering”, redirects it away from the direction under consideration. Energy that is absorbed manifests as an increase in internal energy, whereas scattered energy is redirected.

The total attenuation, or extinction, is the combination of absorption and scattering,

$$
(dl_{\lambda})_{abs} = -\kappa_{\lambda} l_{\lambda} ds
$$

(2.29)
where the $\lambda$ indicates that the equations are spectral and $I$ is the intensity. The negative sign is added since the intensity is being decreased. The intensity can be determined from integrating these equations over a geometric path.

Extinction is the combination of absorption and scattering,

$$dI_\lambda = -(\kappa_\lambda + \sigma_\lambda)I_\lambda \, dz$$ (2.31)

where $z$ is the axis parallel to the direction that photons of light are moving. Integrating this equation yields the following, where $C$ is the constant of integration,

$$\ln I_\lambda = -(\kappa_\lambda + \sigma_\lambda)z + C .$$ (2.32)

Applying the boundary conditions of,

$$I_\lambda = I_o \text{ at } z = 0$$ (2.33)
$$I_\lambda = I \text{ at } z = s$$

yields,

$$\ln I_o - \ln I = -(\kappa_\lambda + \sigma_\lambda)(0) + C - [-(\kappa_\lambda + \sigma_\lambda)s + C]$$ (2.34)

which simplifies to,

$$\ln \frac{I}{I_o} = -(\kappa_\lambda + \sigma_\lambda)s = -(\beta_\lambda)s .$$ (2.35)

Rearranging this equation gives the Beer-Lambert law, from which the extinction coefficient can be calculated from if the initial and final intensities are known,
Here the extinction, absorption, and scattering coefficients are $\beta$, $\kappa$, and $\sigma$ respectively. The transmissivity, $\tau$, is the ratio of the intensity transmitted through the thickness, $I$, to the incident intensity $I_o$. The thickness or path length is represented by $s$ in equation.

The optical thickness, $\tau_L$, expresses the quantity of light removed from passing through a medium. Based on extinction it is defined as,

$$
\tau_L = \int_0^s \beta \eta \, ds
$$

or

$$
\frac{I}{I_o} = \exp(-\tau_L).
$$

2.4 A Cylindrical Geometric Model

Salita [39] developed a semi-analytical radiation model for cylindrical combustion chamber geometries which can approximate the reacting jet. The radiative flux to a cylindrical wall surrounding a gas/particle mixture having a uniform density, $\rho_m$, and a particle temperature $T_p$ is defined as,

$$
\dot{Q} = \int_0^\infty \tilde{E}(\lambda, \eta, T_p, T_w) \left[ R_{\lambda b}(\lambda, T_p) - R_{\lambda b}(\lambda, T_w) \right] d\lambda
$$

where,

$$
\tilde{E} = \frac{E}{1 + \left( \frac{1}{E_w} - 1 \right) E}.
$$
Here the terms $R_w$, $T_w$, and $E_w$ are the radius to, temperature of, and emissivity of the wall. $E$ is the hemispherical emissivity of the cloud and $\lambda$ is the wavelength of the thermal radiation.

The spectral radiancy, $R_{\lambda b}$, is determined from Planck’s law,

$$R_{\lambda b} = \frac{C_1}{\lambda^5 \left[ \exp \left( \frac{C_2}{\lambda T} \right) - 1 \right]} \quad (2.41)$$

where $C_2 = 1.4388 \text{ cm-K}$, and $C_1$ is determined using the Stefan-Boltzmann constant as follows:

$$\sigma = \frac{C_1 \pi^4}{15C_2^4} \quad (2.42)$$

Integrating over a bandwidth from $\lambda_1$ to $\lambda_2$, while assuming that $E$ is piecewise constant over this range, the radiative heat flux can be expressed in terms of the effective (engineering) emissivity,

$$\dot{Q} = \varepsilon \sigma (T_p^4 - T_w^4) \quad (2.43)$$

where the effective emissivity is,

$$\varepsilon = \frac{15}{\pi^4} \sum_{i=1}^{\infty} \sum_{m=1}^{\infty} E_i \frac{T_p^4 S_{im}(T_p) - T_w^4 S_{im}(T_w)}{T_p^4 - T_w^4} \quad (2.44)$$

and represents the gray emissivity over the range $\lambda_1$ and $\lambda_2$. Here,

$$E_i = E \left( \frac{1}{2}(\lambda_{i+1} + \lambda_i), r, T_p, T_w \right) \quad (2.45)$$

$$S_{im}(T) = A_m \left( \frac{C_2}{\lambda_{i+1} T} \right) - A_m \left( \frac{C_2}{\lambda_i T} \right) \quad (2.46)$$

$$\lambda_i = (i - 1) \Delta \lambda \quad (2.47)$$
\[ A_m(z) = (m^3z^3 + 3m^2z + 6mz + 6) \frac{e^{-mz}}{m^4} \] (2.48)

and

\[ z_i = \frac{C_2}{\lambda_i T}. \] (2.49)

For a cylindrical medium:

\[ E_i(\lambda, T_p) = \frac{4k}{2k + 3 \frac{I_0(k\tau)}{I_1(k\tau)}} \] (2.50)

where,

\[ k = \sqrt{3(1 - \omega)} \] (2.51)

\[ \omega = \frac{K_s}{K_a + K_s} \] (2.52)

\[ \tau = (K_a + K_s)R_w \] (2.53)

and \( I_0 \) and \( I_1 \) are modified Bessel functions.

For \( \tau \gg 1 \) the solution reduces to that for a slab (see Florko et al. [37]):

\[ E_i = \frac{4k + G}{2k + 3} \] (2.54)

where,

\[ G = 3 - \frac{6}{k} + \left( \frac{6}{k^2} - 2 \right) \ln(1 + k). \] (2.55)

When \( \tau \ll 1 \),

\[ E_i = 2(1 - \omega)\tau. \] (2.56)
Effective emissivities are plotted in Figure 2.10 for a range of particle temperatures and for a cylindrical radius of 0.0254 μm (the inner radius of the linear test combustor). Cloud emissivities of 0.1 (for a cloud density of 200 g/m³ of particles) have been reported by Florko et al. [37] and are plotted in Figure 2.10. In this figure the point at 0.5 μm is for a mixture density of 0.2 kg/m³, whereas the solid lines represent $\rho_{\text{mix}} = 0.28$ kg/m³. Finally Figures 2.11 and 2.12 show predictions of anticipated UV and visible light flux as a function of MgO temperatures and cylinder radii.

![Figure 2.10: Spectral Emissivity in a Particle Cloud](image)

Figure 2.10: Spectral Emissivity in a Particle Cloud
Figure 2.11: Predicted UV and Visible Flux for 0.1 μm MgO

Figure 2.12: Predicted UV and Visible Flux for 1 μm MgO
2.5 Chemical Equilibrium Estimation of Flame Temperature

The computer program SOLGASMIX [40] was used to calculate the adiabatic flame temperatures of the Mg-air chemical reaction. The program was designed for calculating thermodynamic equilibrium in complex chemical systems, and has been modified to access a database of thermochemical curvefits. It implements a free energy minimization algorithm.

A system is said to be at its equilibrium state if its composition is resistant to fluctuations of composition and is independent of time and the previous history of the system. An equilibrium analysis may be helpful when the rates of change (reaction and mass transfer) are relatively rapid. There are two general methods of calculating equilibria. The “classical” method uses equilibrium constant expressions to develop a set of nonlinear algebraic equations. These are then solved for the concentrations of various species present. The second determines the equilibrium composition by finding conditions under which total system free energy is minimized. The classical method is well suited for hand calculations whereas, the direct free energy minimization method is appropriate for implementation on a computer as an iterative process.

The total free energy of a chemical system is given by,

\[ G_s = \sum n_i (\Delta G_i + RT \ln a_i) \]  \hspace{1cm} (2.57)

Here \( \Delta G_i \) is the standard free energy of species \( i \) at temperature \( T \), \( R \) is the gas constant, \( n_i \) is the molar amount of species \( i \) and \( a_i \) is the activity of the species. In dimensionless form, the total Gibbs free energy of an ideal system containing gaseous phase, condensed mixtures, and pure condensed species is express as,
\[
\frac{G_s}{RT} = \sum n_i \left( \frac{\Delta G_i}{RT} + \ln P + \ln \frac{n_i}{N} \right) + \sum \sum n_i \left( \frac{\Delta G_i}{RT} + \ln \frac{n_i}{N} \right) + n_i \left( \frac{\Delta G_i}{RT} \right) \tag{2.58}
\]

where \( N \) is the total number of moles of all species in a mixture. The molar amounts of each element must be conserved, constraining the solution by,

\[
\sum n_i A_{ij} = b_j \tag{2.59}
\]

where \( A_{ij} \) is the coefficient on element \( j \) in the formula of species \( i \), and \( b_j \) is the number of moles of element \( j \).

The SOLGASMIX program uses Lagrange’s method for multipliers and a Taylor series expansion, along with the following relationship for Gibbs free energy,

\[
\Delta G_i = \Delta H_i - T \Delta S_i \tag{2.60}
\]

with the enthalpy being,

\[
\Delta H_i = \Delta H_i^\circ + \int_{298K}^{T_o} C_{p,i}(T) dT - \sum A_{ij} \int_{298K}^{T_o} C_{p,j}(T) dT \tag{2.61}
\]

and the entropy as,

\[
\Delta S_i = S_i^\circ + \int_{298K}^{T_o} \frac{C_{p,i}(T)}{T} dT - \sum A_{ij} \left( S_i^\circ + \int_{298K}^{T_o} \frac{C_{p,j}(T)}{T} dT \right). \tag{2.62}
\]

Here \( C_p \) is the specific heat, \( T_o \) is the temperature for which the value of \( \Delta G \) is to be evaluated, \( \Delta H_i^\circ \) is the standard free energy of formation for species \( i \) at 298K, and \( S_i^\circ \) is the absolute entropy. SOLGASMIX predicts the heat of reaction by calculating the integral terms in the above equations. It also finds the heat released by reaction process from,
where $Y_i$ is the number of moles of each product present at equilibrium and $X_i$ represents the starting amounts of each reactant.

SOLGASMIX was interfaced with the JANNAF curvefit database by Peters [40], which contains tabulated data for a number of thermochemical functions, including specific heat and Gibbs free energy values. There are several limitations to the program mentioned by Peters [40]. Chemical reactions with very slow rates, high activation energies, ones that cannot reach equilibrium without catalysis, and processes dependant on the mixing of chemical species are cases where an equilibrium analysis could disagree with observed results.

This computer program was used to predict the adiabatic flame temperature for different air to fuel molar ratios at a pressure of 1 atm. The combustion of magnesium in air can be written as,

$$Mg + n[O_2 + 3.76N_2] \rightarrow \text{Products}.$$

The SOLGASMIX code computed the adiabatic flame temperature for various values of the mass air to fuel ratio, which is shown in Figure 2.13. The original curvefit database only contained temperatures up to 2000 K, and the program would attempt to extrapolate to higher temperatures thus producing the erroneous results depicted by the red squares/line in the figure. Since this is much lower than what is expected from magnesium combustion in air, the computer program had to be updated by Peters (personal communication) to include data at higher temperatures.
Figure 2.13 shows the difference between the adiabatic flame temperatures calculated by both versions of the computer program. It also displays the range of melting point temperatures for MgO. The melting point of MgO is reported to be between 3050K and 3250K [41, 42]. The highest temperatures estimated by the SOLGASMIX code are around 3105K, just inside the range of MgO melting temperatures. If no dissociation occurs, then one would expect that the predicted adiabatic flame temperature curve peaks at a molar air to fuel ratio, $n$, of about 0.5. This is a chemically balanced stoichiometric mixture represented by,
\[ Mg + \frac{1}{2} [O_2 + 3.76N_2] \rightarrow MgO + \frac{3.76}{2}N_2 \]  

where all the oxygen and magnesium is used during the reaction to form the products. Therefore the highest adiabatic flame temperature corresponds to the chemically balanced reaction. As the ratio increases, there is more air than magnesium, and the adiabatic flame temperature decreases. However, the SOLGAS MIX program also computes the molar amounts of the dissociated products produced by magnesium combustion. The effect of dissociation is to push the location of maximum temperature to the left in Figure 2.13. With dissociation, the maximum adiabatic flame temperature occurs for an air/fuel mass ratio of 0.3. The amounts for various species are plotted in Figure 2.14 relative to one mole of magnesium reactant. The region in Figure 2.14 where both solid and liquid phase MgO exist correspond to the maximum temperature (i.e. the MgO melting point). The very rapid reduction in temperature for air/fuel > 1 occurs because of the formation of monatomic oxygen and NO.

![Figure 2.14: Molar Amounts of Product Relative to the Initial Mg Amount](image-url)
Figure 2.15 summarizes several studies of temperature measurements found for various pressures completed by Florko and Golovko [20], Pokhil et al. [43], and Gusachenko et al. [44]. These studies also determined the temperatures for several different oxidizer to fuel ratios. At atmospheric pressure the temperatures reported by Figure 2.15 are comparable to those found by the SOLGASMIX code for the same air/fuel ratios.

![Figure 2.15: Previous Findings of Temperature as a Function of Pressure and n](image-url)
Chapter 3: Calibration of Measurement Method

3.1 Equipment

A linear test combustor that was developed at the ARL for metal aerosol combustion research was used with different optical hardware during combustion testing. The optical hardware consists of six spectral collimators, custom FiberView fiber optic cables, a spectrograph with a CCD camera that allows data to be saved on a computer, and UV sensitive silicon diode photo-detectors.

3.1.1 Linear Combustor

The linear combustor was previously designed and built for use with metal particle fuels and to measure combustion parameters, was used for this testing. Its design allows the fuel type, particle size, oxidizers, fuel concentrations/particle cloud densities, and other combustion parameters to be varied. This combustor is 2 inches in diameter, 40 inches long and consists of three axial, removable sections with a total of fifteen separate view ports, shown in Figure 3.1. An inner graphite liner is present that is capable of withstanding the intense heat produced when combusting metals. Outside of this liner there is a water-cooled structural wall that helps provide cooling as needed.
Access ports are located regularly along the combustor length to permit thermocouple, pressure transducer, and optical access. Figure 3.2 shows a cross sectional drawing of the linear combustor and a view port. Two different types of instrumentation were used to record data during testing. The silicon diode photo-detectors express a measurement of light intensity as a voltage output. Collimators and fiber optic cable were used to view the spectral distribution of intensity output.
3.2 Calibration Bulbs

For the purpose of calibration, two standard-grade light bulbs were used with a special calibration setup. This setup, shown in Figures (3.3 and 3.4), consists of the calibration lamp and fixture. The fixture is an access port, like those found on the linear combustor, which is mounted on a black plate. The instrumentation, either a collimator or silicon diode, can be placed in this port and the fixture can be moved to different distances away from the light source. Specific distances correspond to different flux values. The lamp holder has been constructed to reflect a negligible amount of radiant flux so as not to add to the output readings. The shape factor effects were determined from testing with this calibration stand.
Two light sources were used during calibration. A Standard of Color Temperature, OL 200K, S/N: S-1059 and a Standard of Spectral Irradiance, OL 200C, S/N: S-01058. These lamps are commercial G.E.
type DXW 1000-Watt lamps having a tungsten coiled-coil filament enclosed in a small quartz envelope. These calibration lamps were used in the calibration setup shown in Figure 3.3.

### 3.2.1 Standard of Spectral Irradiance

The Standard of Spectral Irradiance lamp was used to calibrate the emission measurement. Figure 3.5 shows a table taken from the Optronic Laboratories, Inc. Report of Calibration [45]. This table shows the predicted spectral irradiance output of the Standard of Spectral Irradiance lamp over a wavelength range. The total irradiance is based on the radiance of a black-body defined by the Stefan-Boltzmann radiation law, which was discussed earlier in Chapter 2. The assigned values of total irradiance, found in Figure 3.5, have estimated uncertainties of ±1%. These values are based on the National Bureau of Standards scale of spectral irradiance. This was demonstrated at a distance of 50 cm and a current of precisely 8.00 amperes DC flowing through the lamp.

### 3.2.2 Standard of Color Temperature

The Standard of Color Temperature data from the Optronic Laboratories Inc. [46] is found in Figure 3.6, and was used in order to calibrate the temperature measurement. This table shows the color temperature of the source at varying currents. As the lamp current is increased, the corresponding color temperature also increases. The estimated uncertainty in the color temperature calibration is ±20 K. The lamp sources were used in the calibration stand at a distance of 50 cm and inside the linear combustor. This 50 cm distance was measured from the bulb filament to the detector that was measuring output. The spectral irradiance standard lamp was also used insitu the combustor to mimic the combustion and enable assessment of optical port view factors. The calibration lamp in Figure 3.7 is shown shining through a view port for calibration purposes.
Figure 3.5: OL200C Calibration Report

<table>
<thead>
<tr>
<th>Wavelength (nm)</th>
<th>Spectral Irradiance (μW/cm² nm)</th>
<th>Wavelength (nm)</th>
<th>Spectral Irradiance (μW/cm² nm)</th>
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Project No: 967-732  
Calibration Date: May 21, 2002  
Certification Date: May 31, 2002
### Table 1

Color Temperature versus Current for Standard S-1059 at 10 K intervals.

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Project No: 907-732  
 Calibration Date: June 3, 2002  
 Certification Date: June 3, 2002
3.3 Instrumentation

3.3.1 Silicon Diode Photo-Detectors

The four silicon diode photo-detectors transformed light (specifically UV) energy into an electrical current through the photovoltaic effect. These (IFW/JIC138) detectors have a specific sensitivity in the UV spectral range of 210-390 nm. Figure 3.8 is a photograph of the silicon diode detectors, which shows their relative size. The relative spectral responsivity provided by the manufacturer is shown in Figure 3.9. The diodes are most responsive around a wavelength of 280 nm.
Figure 3.8: Silicon Diode Detectors

Figure 3.9: Published Silicon Photo-Detector Responsivity
The silicon diode photo-detectors were calibrated by exposure to the Standard of Spectral Irradiance lamp previously described. The silicon diode photo-detectors were placed in the calibration fixture and given an open view of the bulb with a view factor of 1.0. Readings of the voltage at different distances from the light source were recorded in Table 2. This was done at a lamp current of 8.0A with the OL200C calibration bulb. Following the general calibration procedure, the photo-detectors were then mounted in a fixture that mimics the view factor that exists in the optical access port of the combustor (see Figure 3.4). Finally the UV absorbance by the quartz lenses separating the exterior of the optical access ports from the internal combustor was also measured and found to be 10%.

Table 2: Silicon Detector Calibration

<table>
<thead>
<tr>
<th>Distance (cm)</th>
<th>SD #1 (Volts)</th>
<th>SD #2 (Volts)</th>
<th>SD #3 (Volts)</th>
<th>SD #4 (Volts)</th>
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<td>0.104</td>
<td>0.096</td>
<td>0.144</td>
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<td>30</td>
<td>0.272</td>
<td>0.297</td>
<td>0.272</td>
<td>0.41</td>
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<tr>
<td>15</td>
<td>1.12</td>
<td>1.182</td>
<td>1.101</td>
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<td>No Light</td>
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<td>0.003</td>
<td>0.002</td>
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Table 3 shows the published spectral irradiance for the OL200C calibration lamp and the filtering factors from Figure 3.9. From these values the actual spectral emission that is measured by the silicon diode detectors in the 210 to 390 nm range was calculated. This table also shows the calibration factors.
that can be used to convert the diode voltage measurements into the amount of UV that was emitted.

Two calibration factors were determined, one for the broadband spectrum and the other for the UV region. These values were calculated from,

$$f_{calibration} = \frac{Total\ Spectral\ Emission}{Measured\ Output}. \quad (3.1)$$

### Table 3: Silicon Diode

<table>
<thead>
<tr>
<th>Wavelength nm</th>
<th>OL200C S-11058 Irradiance @ 50 cm $\mu$W/cm$^2$-nm</th>
<th>Bulb Spec Emis $\mu$W/cm$^2$</th>
<th>JIC 137 Filtering SD</th>
<th>Measured SD Spec Emis $\mu$W/cm$^2$</th>
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<td>0.53</td>
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<td>270</td>
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<td>0.7</td>
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</table>

| Detector Area | 0.22 mm$^2$ | | |
| Sensitivity   | 1.2 mV/nW  | | |
| Expected Output | 42.5218728 mV | UV | |

| Measured Output | 0.096 V | Unobstructed view of light @ 50 cm distance |
| Cal Factor      | 1248.239583 $\mu$W/cm$^2$/V | Broadband Spectrum |
| Cal Factor      | 167.7788542 $\mu$W/cm$^2$/V | UV Spectrum |
3.3.2 Collimators/Spectrograph System

The spectrograph-based system employs a spectrograph and charge-coupled device (CCD) array to take snapshots of the spectral light signal at up to six different locations along the combustor simultaneously. The camera speed allows for a snapshot to be taken every 2.4 seconds. The spectrum is then recorded using a PC with camera controller and spectrographic software [47, 48]. The layout of this system is shown in Figure 3.10 taken from Moore [13]. An Acton Research Corporation Model MS-416 Pen-Ray Mercury vapor bulb was used to perform the frequency calibration of the camera (see reference [49]) and verified the ability to measure in the UV spectrum.

![Figure 3.10: Layout of the Optical Diagnostics](image)

The six collimators, four of which are shown in Figure 3.11, can be inserted into the viewports outside the quartz windows to measure the intensity produced. The process starts when light from the combustion reaction passes through the viewport and quartz window to reach the collimator, which
focuses the light onto the inlet of a single optical fiber. This custom cable consists of six fibers and was manufactured in order to properly capture the ultraviolet range. The light then passes through the fiber to the inlet of the spectrograph to a filter just in front of the spectrograph slit. Once passing through the slit, the light travels into the spectrograph where it is split to give a full spectrum over the wavelength range. The data is saved as a gray body curve from which the color temperature and spectral irradiance of the combusting particles can be determined. Normally these collimators are not sensitive to UV; the present devices were coated by the vendor with Lumogen to enable UV sensitivity.

![Collimators with Fiber Optic Cable](image)

**Figure 3.11: Collimators with Fiber Optic Cable**

Figure 3.12 is a drawing of the custom optical fiber cable. The cable splits into the six separate fibers at the end where the collimators can be attached. The diagram also shows the internal cross...
section of the cable. Here the six fibers are aligned in a vertical line. Fiberguide fiber optic cables were used in this study, again for the purpose of enabling UV measurements.

Figure 3.12: Optical Fiber Drawing

The transmission of the UV and visible spectrum of the fiber optic cables is displayed in Figure 3.13. The cable used in this work was 0.75 m and therefore the attenuation is similar to the Superguide PCS 0.5 m length cable shown in the graph. According to this figure, the cable is transmitting from 30% to 46% in the UV and visible range, respectively. Although low, this level of sensitivity should still enable measurements of relative quantities like absorption.
3.3.3 Instrument Setup

Both the silicon diode detectors and collimators can be used in the view ports during the same test. Five view ports on the top of the linear combustor were adapted and used for the bacteria solution while the six side view ports were used for other instrumentation as shown in Figure 3.14. The silicon diodes are placed on top of the sample to measure the amount of UV flux that passes through the sample. A schematic from the top of the linear combustor setup displaying the locations of the six fiber optic cables with collimators and the silicon diode detectors is shown in Figure 3.14. Optical fibers 3 and 4 view the same location from opposite sides and should record similar data. Solution samples were inserted in view ports #2-5 with silicon diode photo-detectors placed in each one.
Figure 3.14: Instrumentation Locations, Top View of Linear Combustor

Figure 3.15: Placement of Biological Sample
Figure 3.15 illustrates the placement of a sample that may contain a particulate suspension or just the suspension liquid. The samples can only be inserted in the vertical viewports on the top of the combustor. These access ports have been modified with o-rings in order to make the cavity water tight. As shown in the figure the sample rests directly on top of the quartz window and a silicon diode detector or collimator can be placed above it to measure the UV that is transmitted through the solution. The broadband attenuation of UV by the windows was measured and accounted for during testing and found to be ~10%.

Figure 3.16: Combustion Testing Setup
Figure 3.16 is a photograph of the setup during the combustion testing. It shows the collimators and silicon diode detectors already inserted into the proper view port locations. Note that this photo is backwards of that in the schematic (Figure 3.14), with the igniter being on the right hand side. Here the flow through the combustor travels from right to left.

3.4 Collimator Calibration

The spectrograph capability, including collimators, fiber-optics, and CCD camera was calibrated using a mercury vapor Pen-Ray light source, for which the relative intensities at specific wavelengths in the UV are known. Following the calibration guide, the lamp was mounted directly to the entrance of the entrance slit. Figure 3.17 shows the spectral measurements at different stages of Mg combustion. Note how well the UV Mg emission spike spectral location and relative strength are measured. The specifics of the combustion test that generated these plots follow.

![Figure 3.17: Measured Magnesium Combustion Spectrum](image)
The spectrograph setup was used with the six collimators and custom manufactured optical fiber cable. The collimators were tested with a fluorescent light source to assess sensitivity in the near-visible and visible ranges. Figures 3.18 and 3.19 are the published and experimental sets of data respectively. Figure 3.18 shows twenty-two peaks between 400 nm and 815 nm. This is for a typical modern fluorescent lamp, which is the most common type.

![Image of Figure 3.18: Intensity of Spectral lines of a Modern Fluorescent Lamp [Wikipedia]](image)

The spectrum of a typical fluorescent lamp that was measured by the spectrograph is shown in Figure 3.19 and is comparable to that of the reported data. The three greatest peaks (4, 5, and 12) were found at similar wavelengths. A clearly defined double peak was recorded around 550 nm.
Overall most of the spectral peaks in Figure 3.18 can be observed in the measured data. When zoomed in the smaller peaks that were close together can be observed. Figure 3.20 is the spectrum over a smaller range of wavelengths. Here the peaks 6-11 can be detected.
The peaks of 13 and 14 cannot be picked out. The large peak at 600 nm (# 12) has a steeper slope in the published data than in the recorded spectrum. In the measured spectrum the peaks at 13 and 14 cannot be distinguished due to this larger peak, since there was not enough resolution.
3.5 Optical Temperature Measurement Methods

3.5.1 Pyrometry

One of the first and most conceptually simple optical temperature measurement techniques is based on the use of the Stefan-Boltzmann law and the gray body approximation:

\[ Q = \varepsilon \sigma T_p^4 \]  

(3.2)

From a measurement of the emitted flux AND a good estimate of the effective emissivity, a combustion zone temperature can be inferred. For Mg combustion, values of emissivity, \( \varepsilon \), from 0.1 to 0.3 have been advocated (Florko et al. [37] and Newman and Payne [23]). The fact that a good prior knowledge of this property is required, compromises the accuracy of the method. Newman and Payne [23] describe how the flame temperatures they measured in this way were subject to errors due to the flame not being optically thick, as well as, incomplete knowledge of the emissivity. Specifically, the measured pyrometrically-based color temperatures of ~3900 K when the adiabatic flame temperature limit was ~3100 K.

To alleviate some of this uncertainty, two- and three-wavelength pyrometric techniques have been developed. For a combustion zone temperature that is much greater than the ambient temperature, and assuming that the effective emissivity is a function of wavelength, the following relation between spectral emissivity and the spectral flux exists (see Dreizin and Hoffman [50]):

\[
\frac{E_{\lambda_1}}{E_{\lambda_2}} = \left( \frac{\lambda_1}{\lambda_2} \right)^5 \frac{\exp \left( \frac{C_2}{\lambda_2 T} \right) - 1}{\exp \left( \frac{C_1}{\lambda_1 T} \right) - 1}.
\]  

(3.3)
The benefit of this method is that the magnitude of the emissivity at the two target wavelengths are not needed, only the RELATIVE spectral flux intensities at those locations are. Pokhil et al. [43] indicated a ~400 K error in their aluminum-based temperature estimates.

Driezen et al. [15] applied a three wavelength pyrometry technique to aluminum combustion. Relative radiated intensities at 458, 520, and 580 nm were chosen. His calibration indicates that at two intensity ratios; \( \frac{I(580 \text{ nm})}{I(520 \text{ nm})} \) and \( \frac{I(580 \text{ nm})}{I(458 \text{ nm})} \), could be used to generate +/- 80 K accuracy for measurements in the 1900 – 3273 K range.

### 3.5.2 Resonance Line Reversal Method

Moore et al. [13] adopted the resonance line reversal method (Alkemade [51], Graydon and Wolfhead [52], and Pokhil et al. [43]). In their work, light from the Oriel 6317 source lamp (used for the temperature standard in the present thesis) passed through two lenses so that the filament of the lamp was in focus above the flame (Moore was studying a stationary flame over a liquid metal pool). The combined image of the filament and flame was focused on the slit of the Acton Sp-306 spectrograph and then dispersed by the CCD array (both instruments were used for measurements in the current thesis). The lamp temperature was adjusted until a resonance line for the flame temperature was reached. The cross-over point between emission and absorption was readily determined. Note that Moore used this method for lithium flame temperatures while Pokhil et al. [43] measured aluminum flames (these measurements were closer in agreement than their two- wavelength pyrometric measurements and ~300 K in estimated error). Florko et al. [53] applied this method to a Mg particle reacting with oxygen. They measured maximum temperatures in the range of 2630 to 2750 K, and claimed an experimental error of +/- 30 K.
3.5.3 Planck’s Law Method

Moore et al. [13] applied a technique based on an evaluation of the continuous emitted spectrum to predict the optical standard bulb temperatures. By matching a large section of their measured spectrum to predictions made using Planck’s law using an algorithm that produced a least squares minimization based on varying overall emissivity and combustion temperature. A very similar method was developed and used independently by Pokhil et al. [43] (though using Wien’s approximation of Planck’s law). Their inferred error was ~300 K; which was less than that reported for their two-wavelength pyrometric method. This method was chosen for use in the work described here because of the following reasons:

1. The measurement instrumentation, advice, and methodology were readily available
2. A good estimate of color temperature was not required
3. A complicated optical setup was not required
4. Temperature measurements were estimated to be as accurate as by any other method.

The collimators with the six fiber optic cables were each tested individually with the same OL 200C calibration light source to observe the difference between fibers. The results are shown in Figure 3.21, where the solid black line is the Planck’s law curve, and the other curves represent measurements by each collimator/fiber optic cable and of the emission produced using the voltages prescribed in the calibration report of Figure 3.5. The 620 nm to 750 nm range is the one of interest since this is where the slopes of the theoretical Planck curve and the experimental measurements match. The fiber optic cable that was used for Moore’s previous work in the 470-1000 nm range is also shown in Figure 3.22 as the blue dashes. As seen in the figure, this fiber optic cable was not designed for use in the UV range and cannot pick up wavelengths less than 470 nm.
The Standard of Color Temperature light source was used in the calibration setup with the collimator at a distance of 50 cm away. Following the calibration report in Figure 3.6 the various currents were used to determine the relation to temperature. The published current values were inputted into the programmable DC current source and the data was plotted in Figure 3.22.

A Microsoft Excel spreadsheet tool was employed to home in on a correct temperature and emissivity. This solver uses a least squares optimization to fit a Planck’s law curve to a specific region of the measured data. The emissivity and temperature are changed until the values that produce the lowest root mean squared error between the two curves are found.
The Excel solver was used with the gray body curves recorded from Color Temperature light source and the results are plotted in Figure 3.22. Using Planck’s law and the temperature corresponding to the specific currents produced the smooth lines in this figure. The experimental data and the Planck’s law slopes match up very well in the area of interest of 620 nm to 750 nm. That a Planck’s law estimation is valid in this region is consistent with Florko and Golovko’s [20] measurements of spectral emissivity which show a constant gray body emissivity for wavelengths greater than 600 nm (and less than ~850 nm – the limit of their measurements).
The Excel solver was able to predict the temperature within 14-66 K, with a percentage error ranging from 0.62% to 2.1%. These errors and difference in temperature are found in Table 4. As the temperature is increased so is the error.

<table>
<thead>
<tr>
<th>Accepted Temp (K)</th>
<th>Predicted Temp (K)</th>
<th>ΔT</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000</td>
<td>2016</td>
<td>-16</td>
<td>0.8</td>
</tr>
<tr>
<td>2250</td>
<td>2236</td>
<td>14</td>
<td>0.622222</td>
</tr>
<tr>
<td>2500</td>
<td>2478</td>
<td>22</td>
<td>0.88</td>
</tr>
<tr>
<td>2800</td>
<td>2767</td>
<td>33</td>
<td>1.178571</td>
</tr>
<tr>
<td>2900</td>
<td>2863</td>
<td>37</td>
<td>1.275862</td>
</tr>
<tr>
<td>3000</td>
<td>2964</td>
<td>36</td>
<td>1.2</td>
</tr>
<tr>
<td>3050</td>
<td>3010</td>
<td>40</td>
<td>1.311475</td>
</tr>
<tr>
<td>3120</td>
<td>3054</td>
<td>66</td>
<td>2.115385</td>
</tr>
</tbody>
</table>

The data in Table 4 was plotted in Figure 3.23. The figure plots the difference in the calculated and actual temperatures as a function of the reported temperatures. This shows that there is more of a difference between the two as the temperature is increased.
In order to show the uniqueness of the Excel solver solution, figures varying temperature and emissivity were produced. Figures 3.24 and 3.25 show Planck’s law with the 2900 K data that was recorded using the Color Temperature calibration lamp (Figure 3.23). In Figure 3.24 the same temperature of 2900 K was used with higher and lower emissivity, whereas Figure 3.25 uses the same emissivity but different temperatures. These two plots show that the optimized curves produced with the Excel solver are the closest fit to the recorded data. Note that an accurate knowledge of the value of \( \varepsilon \) is not required a priori. The solver homes in on the value that gives the best fit.
Figure 3.24: Same Temperature, Different Emissivity

Figure 3.25: Same Emissivity, Different Temperatures
In Figure 3.26 a point on the measured data was chosen and Planck’s law was calculated using
different temperatures and manually fit to this point by changing the emissivity. Although the different
temperature curves can pass through the given point at 714 nm, they are not the optimal value since
the slopes are clearly different than the measured data.

While short of a rigorous mathematical proof, the results presented here indicate that the
method used here of an automatic least squares optimization as well as the use of a discrete clearly gray
band region for comparison appears capable of accurately predicting the temperature of a reference
temperature standard source. Potentially large over/under estimations of temperature are eliminated
because of the elimination of human subjectivity, and the elimination of the need for a good estimate of
the gray-body emissivity. The principal contributions to temperature measurement produced by the present work are: strong validation of the method by comparison with known standards, use of a relatively small wavelength range to infer temperature, the use of high frequency measurements to infer temperatures, and the development of an automated least squares fitting routine to eliminate subjective errors.

3.6 Measurement of the Extinction Coefficient of a Suspension Subject to UV and Visible Light

Samples of solution with different concentrations of bacteria (particles) were irradiated using the Standard of Spectral Irradiance lamp inside the linear combustor. These concentrations ranged from $10^1$ to $10^9$ bacteria/mL and each sample had a volume of 400 μL, with each specimen being 0.942 cm in diameter and 0.5735 cm in height. The intensity data measured using the spectrograph is plotted in Figure 3.27 for the different concentrations, where phosphate buffered saline or PBS is the solution that the bacteria are suspended in.
This graph shows the measured intensity coming through the sample. This intensity is decreased with the addition of the solution and more so when the bacteria are present. As the concentration is increased there are more bacteria and therefore more of the UV is being absorbed or scattered away from the sensor. The oscillations presented for wavelength greater than 470 nm are a result of optics. They are linearly proportional to intensity, and may be readily eliminated by subtraction of one curve from another. The collimator/fiber-optic system is clearly most sensitive in the near-visible and visible wavelengths. However, smaller amplitude signals in the UV can be distinguished (as shown in Figure 3.28), and the ability to distinguish amplitude in wavelength was shown to be good in Figure 3.17.
The oscillatory behavior at higher wavelengths is due to scattering produced by the liquid media. This is a result anticipated by Mie scattering theory and not a product of the measurement method. As the particle concentration increases the scattering effect reduces.

While this section of the measured spectrum is relatively flat for these measurements, the previously shown ability (shown later in this thesis) to clearly distinguish the 285 nm Mg emission line clearly shows the ability of the collimator and fiber optic system used here to measure in the UV spectrum.
Figure 3.29: Fraction of Light Being Extinguished by the Bacteria in UV Range

Figure 3.30: Fraction of Light Extinguished Over Entire Spectrum
The fraction of UV absorbed as a function of wavelength is plotted in Figures 3.29 and 3.30 for the various concentrations. As the concentration of particles is increased, the amount of UV that is being absorbed is also increased. Since there is a small number of particles in the $10^3$ concentration compared to the volume of solution, this can be treated as the fraction of UV absorbed by the solution for $\lambda < 500$ nm. The large scattering effect can be seen for $\lambda > 500$nm.

The extinction coefficient was calculated for the various concentrations and can be found in Figures 3.31 and 3.32. This coefficient was found using Beer’s law, equation 2.35, with the values of intensity transmitted through the samples and the incident intensity. The $10^3$ concentration has been treated as the absorption of the PBS solution and has been subtracted from the other sets of data to determine the extinction coefficient of the suspended particulate only.
Figure 3.32: Extinction Coefficient of the Particles (Bacteria) Over the Entire Spectrum

Figure 3.32 shows the calculated extinction coefficients for the various bacterial concentrations. The higher the concentration the less intensity coming through the sample. The extinction coefficient also tends to increase over the wavelength spectrum, meaning that less intensity is being let through at the higher wavelengths.
Extinctions coefficients were determined at different wavelengths (243 nm, 300 nm, 360 nm, 400 nm, 500 nm, 600 nm, 700 nm, and 800 nm) and plotted in Figure 3.33 as a function of concentration. This shows that there is a greater difference between the extinction coefficients at different wavelengths as the concentration of bacteria is increased.
The broadband extinction coefficients were also obtained from the silicon-diode photodetector voltage measurements and are plotted in Figure 3.34. The coefficients were calculated for the data taken on different days and are represented by the diamonds in the figure. The very low value at n = 5 was regarded as flawed and therefore was ignored. The fraction of UV absorbed determined from the silicon-diode detectors compares very well to that which was measured from the collimators.
Chapter 4: Testing and Results

4.1 Combustion Setup

The overall setup for the combustion trials was the same as in the calibration testing, except an igniter, fuel feed system and the water cooling system were utilized. The instrument setup shown in Figure 3.14 was used with a video camera in an open side view port to view the combustion. Various other instruments were used in order to measure the pressure and other aspects.

![Linear Combustor Cross-Sectional View](image)

Figure 4.1: Linear Combustor Cross-Sectional View

A drawing of the injection section of the linear combustion is seen in the figure above. The metal fuel is injected into the combustor at the right hand side of the drawing in Figure 4.1. Once it is ignited, the powered magnesium is pushed downstream of the combustor by a flow of argon. A jet of
water is also run outside of the graphite liner to keep the combustor cool. The fuel feed system is shown in Figure 4.2. This metal feed system can inject of dense metal particulate clouds at variable rates for up to 30 minutes.

Figure 4.2: Metal Power Fuel Feed System
The diagrams in Figure 4.3 were used during the combustion testing and show the top and side view of the combustor. These show the locations of instrumentation and were used to observe temperature, pressure, and voltage outputs during the combustion process. The water tank located at the exit of the combustor is visible in the bottom right hand side of the figure.

Figure 4.3: Data Output Schematic
4.2 Combustion Results

4.2.1 Spectral Detection in the UV and Visible Range

Combustion runs for varying times ranging from fifteen seconds to four minutes were made. Voltage measurements were taken by the silicon diode detectors and converted using the calibration factor to UV flux. Also the intensities over the wavelength spectrum were measured. Figure 4.4 shows the intensity measurement in the UV range from one of the first tests. Here five of the fiber optic cables were used to capture the spectrum. The mass flow rates of magnesium and air were 0.003 and 0.01 kg/s, respectively. In this run, a progressive heating occurs between ports 1 and 3. Ignition occurs somewhere between 3 and 4, and combustion tapers down between ports 4 and 5. According to Newman and Payne [23], there is an emission spike for magnesium at 285.21 nm, which corresponds nicely to the experimental data. These results show that the ability for the present collimator system to detect and resolve spectral data in the UV-A range is possible, lending credence to the extinction coefficient results presented in Figures 3.29-3.33.
Figure 4.4: Peak at 285 nm of 45 Second Run

Figure 4.5: Relative Intensity at 285 nm Over Time
The magnitudes of the 285 nm peaks shown in Figure 4.5 are normalized relative to the maximum peak, and plotted at the burn time at which the measurements were made normalized to the time of the peak intensity measurement. This permits an approximate “apples to apples” comparison with the intensity measurements of Valov et al. [16] which were made for a single larger diameter particle. The good agreement between measurements gives some confidence that the relative magnitudes of the spectral UV shown in Figure 4.4 are reasonable.

Figure 4.6 shows spectral measurements corresponding to combustion with magnesium and air flows of 0.002 and 0.01 kg/s, respectively. Figure 4.7 shows similar spectra; measurements performed by Weiser and Eisenreich [54]. Both graphs exhibit peaks at 380 nm and double peaks at 500 – 518 nm. While 500 nm is characteristic of MgO emission, Valov et al. [16] indicate that the 518 nm line is characteristic of Mg and not (as Weiser and Eisenreich suggest [54]) characteristic of MgO emission. However, the MgO and Mg spikes are clearly present, showing that the system is capable of measuring into the high-frequency visible range. In this run, ignition appears to occur by port 2, combustion is fully underway by port 3, and tapering off towards port 4.
Figure 4.6: Experimental Intensity Data of Two Minute Run

Figure 4.7: Published Mg Powder Flame Intensity [54]
4.2.2 Temperature Predictions

Since the combustion of magnesium produces very high temperatures that are difficult to measure directly, the Planck’s law method previously described was used to infer the flame temperature. Recall, this method involved fitting the Planck’s law curve to the measured intensity data in the 620-750 nm range. By using a built-in Microsoft Excel solver, the emissivity and temperature were cyclically changed to obtain the lowest root mean squared error between the gray body prediction and the measured spectral intensity in the range of interest. A sample result is graphed in Figure 4.8. The dashed lines are the Planck’s law curves that were fitted to the measured data, which are represented by the solid lines in this figure.

Figure 4.8: Temperature Prediction from Intensity from 4 Minute Trial
Figure 4.9 shows spectral measurements and Planck’s law comparisons made over a compressed x-axis at a time during a one minute trial with mass flows of magnesium and air equal to 0.0018 and 0.0045 kg/s, respectively. Note that not all of the collimator/fiber lines had gray body correspondence in the 620 to 750 nm range. Fiber 4 showed a clear correspondence in the 490 to 620 nm range instead. The complete collection of graphs for the rest of the runs completed can be found in the Appendix.
Figure 4.10 displays the spectrum recorded by fiber 3 over time for the two minute run. This graph plots several snapshots taken by the CCD camera from frames 63-75. As the combustion moves downstream, closer to the location of fiber 3, the intensity increases which is seen from comparing the magnitude of frame 63 and 65 to that of the later frames. It is also observed that the magnitude of intensity fluctuated with time for the various runs but the slope of the spectrum in the specific range, which was discussed earlier, remained fairly constant. Since it is the slope of this line that is used to determine the temperature, the fluctuations in intensity are not significant when using Planck’s law.

However, a large spike was recorded at roughly 670 nm and can clearly be seen in the frame 75 spectrum of Figure 4.10. Since this spike was in the 620-750 nm, it affects the Planck’s curve fit found
with the Excel Solver and therefore the predicted temperature. Therefore this peak was eliminated, as shown with the frame 71 data. This spike at 670 nm may have originated from the E. coli fluorescence [55].

Figure 4.11: Predicted Temperatures of Different Mg Flow Rates

Figure 4.11 plots the predicted temperatures as a function of flow rate in lbm/s. The collimator location corresponds to those in Figure 3.14. This shows that the temperature tends to increase downstream. This is due to the magnesium combustion taking place further down the linear combustor. Since it was determined that the most intense magnesium combustion was happening closest to view
port #3, the temperatures predicted there are the highest. The values at this view port clearly show that the temperatures are decreasing as the magnesium flow rate increases. When comparing the difference in the magnesium flow rate it is seen that overall the temperature varies inversely. In this figure the gray box is the range of temperatures of the melting point of magnesium oxide.

The predicted temperatures for 0.004 lb/s flow rate are higher than expected. The exact cause of this is unknown, although it is possible that the igniter was accidently left on meaning that the ignition gases were still flowing through the combustor. These extra gases would yield higher combustion temperatures.

The predicted temperatures mostly lie between 2500K and 3500K, which is similar to the adiabatic flame temperatures computed by the SOLGASMIX code. Points illustrating the temperatures corresponding to different air/fuel ratios are also shown in Figure 4.10. Recall, the code predicted a temperature of about 3100 K for a stoichiometric mixture. The melting point of MgO has been reported over a range of 3050 to 3250 K.
Another representation of the predicted temperatures is shown in Figure 4.12. This plots the temperature as a function of time. The overall temperatures stayed fairly consistent over the different timed runs. The CCD camera takes a photograph of the spectrum every 2.4 seconds missing everything in between. This makes a difference, especially in the shorter runs, since the temperatures at those times cannot be predicted. One clear take away is that as the run progressed, the ignition point moved closer to the front of the combustor.

Fibers 3 and 4 are measuring the intensity at the same point along the linear combustor but from opposite sides. The temperatures are expected to be similar since they are at the same location but there is a slight variation. This difference could be from the location of the magnesium combustion inside the combustor since it is not uniform throughout. Also the angle at which the fiber optic cable
was curved for fiber 4 to reach the opposite side of the combustor could have made a difference in the measurements.

From Figure 4.12 it can be seen that early on the ignition is farther downstream of the combustor, since the highest temperatures were measured with fibers 3 and 4. During the longer runs the combustion has time to stabilize and the greatest temperatures are now seen in the middle of the combustor around fiber 2. Since the combustion process is moving inside of the linear combustor the flame may not be exactly aligned with the view port, meaning that the collimators would not be able to properly capture the most intense spectrum.

### 4.2.2 Mass Flow Rates and Broadband UV Flux

The next series of twelve plots show mass flow rates, chamber pressure, and UV flux measured by silicon diode photodetectors for runs of various times. The UV flux is shown for locations 1-4, which correspond to where the samples and silicon diodes were placed (view ports #2-5 respectively). In each of the plots the flow rate of argon is much smaller than that of the magnesium, which shows that not much argon is needed to push the magnesium down the combustor. Also in each of the following graphs, the chamber pressure remains fairly constant throughout the run.
The shortest run conducted was for 15 seconds. Figure 4.13 shows that the greatest UV flux is found downstream at location 4. The UV flux ranged from 100-300 W/m², which is relatively small when compared to the other runs.
The 30 second run (Figure 4.14) had an UV flux of 200-1400 W/m², which is much higher than the 15 second run. Again the most UV flux was seen downstream at location 4. Temporal variations in magnesium flow rate correlate directly with flux.
During the 45 second run, Figure 4.15, not much UV flux was seen from the first two locations. Unlike the other runs, here the highest UV was recorded at location 3, rather than location 4.
The next run, shown in Figure 4.16, was for a duration of 1 minute. Here the UV flux increased moving downstream, with locations 3 and 4 reporting similar flux.
For the 2 minute run, Figure 4.17, there was a strong UV flux peak towards the beginning but then drops off about half way through the run. The peak corresponds to a drop in the chamber pressure,
which is also when the magnesium flow rate reaches its maximum. During the previous runs the chamber pressure averaged about 1.1 atm throughout the entire run. The two minute run saw the chamber pressure start out at a pressure around 1.5 atm and then drop down to 1.1 atm.

Figure 4.18: Mass Flow Rate (lbm/sec) and UV Flux for Four Minute Run
The longest run was for 4 minutes, in which there was a gradual drop off of UV towards the end. There is a dip around 225 seconds into the run but then increases again, seen in Figure 4.18. There are two spikes in the chamber pressure that correspond to the two dips in UV at 225 seconds and the end of the run. These two peaks were the highest of any of the runs, at a magnitude of 2.3 and 1.8 atm.

There are two main features that need to be emphasized. The first is a strong (and not surprising) correlation between increased flow rates of magnesium and increased UV flux for modest flow rate excursions. For too large an excursion, the main flame zone can be located at more or less advantageous positions relative to the optical access ports. The second feature requiring comment is the tendency in some (especially longer runs) for the UV flux to reduce. One cause might be the movement of the primary ignition zone as the combustor heats up. Another cause may be the gradual accumulation of MgO residue on the combustor interior surface of the optical access ports.

The maximum UV flux measured for the various runs is plotted in Figure 4.19. It compares the measured data to that of the predicted values for UV flux at varying temperatures and MgO particle radii. Here the data shows a rough trend of increasing flux with increasing Mg mass flow. The data is well bounded by the theoretical predictions with the 0.1 \( \mu \text{m} \) radius MgO particle between 2600 and 2850 K. The larger MgO particles (1 \( \mu \text{m} \)) at higher temperatures (2800-3100 K) also appear to give reasonable bounding. This also emphasizes the difficulty with measuring at discrete port sites, since the combustion flame is moving during testing.
Throughout testing there was a problem of debris buildup on quartz windows (Figure 4.20). The magnesium oxide, which is the product of magnesium combustion with air, was building up on the quartz window and blocking the view ports. This was most prevalent during the longer runs of a few minutes. The blockage does not affect the temperature and spectral irradiance measurements since these are recorded throughout the run, and are based on the shape and not the magnitude of the curves. The steady drop off of UV flux found in the longer runs could be related to debris build-up on the quartz window. Because of this the quartz windows had to be removed and the view ports cleaned after most runs.
Figure 4.20: Magnesium Oxide Residue on the Quartz Window
Chapter 5: Concluding Remarks

Theoretical predictions of scattering and absorption cross-sections and emissivities were presented for UV and visible radiant emissions from a single reacting particle and also for a cloud of reacting magnesium particles in air. These predictions were also found to compare well to data from published literature. Theoretical predictions of UV and visible flux were made for a cylindrical reacting jet of magnesium particles in air. The extinction coefficients of a particle suspension were determined. Also in this work, theoretical predictions of the adiabatic flame temperature for a magnesium and air reaction from chemical equilibrium were improved upon.

Methods for measuring the spectral UV and visible flux, as well as the broadband UV flux were demonstrated for the combustion of magnesium. A procedure was developed for deriving the flame temperature from spectral flux measurements. The measurement error associated with these types of measurements was determined. Measurements for the broadband UV flux were made for a linear magnesium and air combustor at different air to fuel ratios. This work also presented measurements of the temperature of Mg and air cloud combustion. The measured UV fluxes and temperatures were well bounded when compared to theoretical predictions.

The UV flux was calculated from the voltage output from silicon diodes for several different runs and plotted along with the magnesium mass flow rate. The chamber pressure was seen to be relatively constant throughout all the runs. It was also observed that the highest UV flux was seen at view ports 4 and 5, which is consistent with the location of the most intense magnesium combustion. The magnesium oxide build-up on the quartz windows was an issue and can limit the length of the runs.

In future work, more realistic testing will be completed and will require reacting metal jets in open air. These tests, with a diode detector, will be set at different distances from the flame. From this
the fall off in UV radiation lethality with distance can be determined and a relationship obtained. Figure 5.1 shows a photograph of a test burn of small propellant grains containing a super-stoichiometric amount of magnesium powder. The reaction between the jet of excess magnesium particles and surrounding air causes the greenish yellow flame. This demonstrates the type of flame that can be used in the next phase of testing.

Figure 5.1: Magnesium Particle Jet Flame
Bibliography


Appendix

The following are plots of the intensity data from the combustion tests. The solid lines are the Planck’s curve fits to the data over the appropriate wavelength range. These curves are represented by the temperature in Kelvin found in the legend on each of the graphs. All air flow rates were 0.0045 kg/sec (0.01 lbm/sec), and the magnesium flow rates are shown in the figure captions.

Figure A.1: Day 1 – 45 seconds, Mg mass flow rate = 0.0032 kg/sec (0.007 lbm/sec)
Figure A.2: Day 1 – 2 minutes, Mg mass flow rate = 0.0032 kg/sec (0.007 lbm/sec)

Figure A.3: Day 1 – 4 minutes, Mg mass flow rate = 0.0023 kg/sec (0.005 lbm/sec)
Figure A.4: Day 2 – 15 seconds, Mg mass flow rate = 0.0036 kg/sec (0.008 lbm/sec)

Figure A.5: Day 2 – 30 seconds, Mg mass flow rate = 0.0041 kg/sec (0.009 lbm/sec)
Figure A.6: Day 2 – 45 seconds, Mg mass flow rate = 0.0041 kg/sec (0.009 lbm/sec)

Figure A.7: Day 2 – 1 minute, Mg mass flow rate = 0.0041 kg/sec (0.009 lbm/sec)
Figure A.8: Day 2 – 2 minutes, Mg mass flow rate = 0.0018 kg/sec (0.004 lbm/sec)

Figure A.9: Day 2 – 4 minutes, Mg mass flow rate = 0.0027 kg/sec (0.006 lbm/sec)