Combustion diagnosis for analysis of solid propellant rocket abort hazards: Role of spectroscopy

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Abstract. Solid rocket propellant plume temperatures have been measured using spectroscopic methods as part of an ongoing effort to specify the thermal-chemical-physical environment in and around a burning fragment of an exploded solid rocket at atmospheric pressures. Such specification is needed for launch safety studies where hazardous payloads become involved with large fragments of burning propellant. The propellant burns in an off-design condition producing a hot gas flame loaded with burning metal droplets. Each component of the flame (soot, droplets and gas) has a characteristic temperature, and it is only through the use of spectroscopy that their temperature can be independently identified.

1. Introduction

For most of the deep space probes and some of the landing craft on mars, NASA has used radioisotope thermal generators (RTGs) to power and to provide heat for the proper operations of their instruments. Most launches of these probes have used launchers with solid rocket boosters (SRBs) as the stage before insertion to earth orbit. In the event of an accident, liquid stages can be shutoff and the autodestruct mechanism allowed to burn and/or disperses the liquid propellant. The fragments of the solid propellant will continue to burn and drop to the ground with a risk of falling near or even on top of the RTG. The main concern is the maximum temperature from the plume impinging on and potentially breach the RTG.

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2. Experimental Setup
Sandia was tasked with measuring the temperatures of a solid propellant plume in an off-design situation. The objective was to define the thermal-chemical-physical environment in and around a plume formed from a burning fragment of solid rocket fuel at atmospheric pressure. Figure 1(a) shows an off-design test burn at Sandia. Figure 1(b) shows three analysis volumes where different chemical dynamics are expected: Region I where the aluminum and the ammonium perchlorate from the propellant burn. Region II is populated by hot emitting gases: hydrogen chloride (HCl), carbon dioxide (CO$_2$), and water (H$_2$O). In this region some burning particles like aluminum monoxide (AlO), alumina (Al$_2$O$_3$), and other particles exist. Region III is where the flame from the plume will most likely interact with the hazardous material in the payload. This situation could lead to more complex interactions in Region II if there is a breach and subsequent release of plutonium-238.

![Figure 1](image_url)

**Figure 1.** (a) Downward setup for off-design burn of solid propellant (b) the plume in the analysis is divided into three regions: I - where aluminum and ammonium perchlorate burn; II - populated by hot emitting gases (HCl, CO$_2$, H$_2$O) and particles(AlO/ Al$_2$O$_3$, etc.); III - where flame will most likely interact with the hazardous material in the payload.

To obtain a better picture of the temperatures seen in the propellant plume, several spectrometers were fielded to measure emissions from the gases (CO$_2$, H$_2$O, and HCl) and alumina (AlO). Two angle-scanning spectrometers were placed orthogonally to each other, to measure CO$_2$ and H$_2$O; one Fourier transform infrared (FTIR) spectrometer measured for HCl; and a grating snapshot fiber connected spectrometer measured AlO emissions.

3. Experimental complexity
The solid propellant burn will generate multiple gases from the reaction of the ammonium perchlorate (NH$_4$ClO$_4$), including CO$_2$, H$_2$O and HCl. The gas temperatures should be lower than the temperatures associated with the burning of aluminum particles as seen in Figure 2. It is expected that the temperatures from the soot will be lower than the temperatures of the gasses and the AlO.
Figure 2. Region I shows the burning aluminum and ammonium perchlorate. Multiple temperatures are present in Region II, complicating measurement and models. AlO is believed to have some of the highest temperatures in this region. Other oxides may be present but they are not being measured. The smoke and soot (non-aluminum related) have the lowest temperature in Region II, probably conforming to a grey body profile. The gases (CO$_2$, H$_2$O, and HCl) fall in the middle of temperature ranges.

4. Aluminum monoxide particles
To observe AlO optical emission spectra from the plume, a probe was inserted into the flame so that specific regions of the plume could be observed. The experiments were performed in a 6.6 by 6.6 meter chamber at ambient conditions, i.e. atmospheric pressure and temperature, analogous to those of an aborted launch. The probe consisted of a steel pipe attached to a stepper motor that moved in regular intervals. One end of the steel pipe was inserted into the plume while a collimating lens coupled to a bifurcated fiber optic cable was attached to the other. Optical emission spectra were recorded with two Ocean Optics fiber spectrometers. One of the spectrometers (HR2000) had narrowband sensitivity in the UV wavelength region of 420-560nm while the other (HR4000 CG) had broadband sensitivity in the wavelength region of 200-1100nm. The average resolution was 0.5nm for the narrowband spectrometer and 0.75nm for the broadband spectrometer. The purpose of the narrowband instrument was to collect aluminum monoxide emission spectra to infer the temperature of the diffusion flame surrounding aluminum particles in the propellant plume. The purpose of the broadband instrument was to collect thermal continuum radiation from the propellant plume to infer the flame temperature. The amount of distance traversed by the steel pipe varied from test to test. Distances from the edge of the propellant ranged from 7.6cm to 38.1cm, with an average spacing between measurements of approximately 0.25cm. To infer the temperature of the propellant plume from optical emissions, aluminum monoxide spectra were fit to theoretical calculations of the AlO spectra and the continuum thermal radiation was used to infer the temperature of the flame.

4.1. AlO results

Figure 3. Fit to experimental AlO propellant spectra.

Figure 4. Planck fitting results for a downward burning propellant.
To infer the AlO temperature, the experimental spectra are fit to theoretical calculations of the AlO $B^2\Sigma^+\rightarrow X^2\Sigma^+$ transition. The theoretical AlO spectra are calculated from accurately compiled line strength tables [1, 2]. The line strength is a popular method for calculating diatomic spectra given the symmetric nature of the quantity. The line strength is also easily calculated in a factorized form from the electronic transition strength, Hönl-London factors, and Franck-Condon factors [3]. The comparisons between experimental and theoretical spectra are made with the use of a Nelder-Mead algorithm. The Nelder Mead algorithm is an optimization technique in which a geometric simplex is created and reduced in size until a specified tolerance level is reached [4, 5]. In order to fit AlO spectra from downward burning propellants, the parameters to be minimized were the temperature, the spectral resolution, and a variable baseline offset. Quadratic baseline offsets were considered for all fits and were found to be linear in nature. This is expected given the AlO emissions are superimposed on thermal continuum emissions and the wavelength region of the AlO emissions. Though the spectral resolution is a largely determined quantity, it was varied to determine the error of the AlO temperature. Though both spectrometers recorded AlO emissions, the narrowband instrument was the primary source for AlO temperature inferences. Values of 0.35 and 0.65 nm were used to over- and underestimate the resolution of this instrument and were corroborated by allowing the algorithm to determine the best possible resolution. A sample fit of AlO spectra is shown in Figure 3 and corresponds to downward burning propellant on a graphite substrate. The measurement was made 7.6 cm from the propellant edge. The inferred temperature for this position was 2969 ± 93K. Typical AlO temperatures were found to be in the 2700-3000K range with typical errors of 95-115K.

4.2. Planck fitting

The temperature of the flame is determined from spectroscopic measurements of the propellant plume and is inferred from broadband emissions in the 500-950 nm wavelength region. The region of analysis is determined from the sensitive range of the broadband spectrometer which was primarily used to infer the flame temperature. The thermal emissions are expected to follow Planck’s radiation law and are considered with various emissivity models. The emissivity describes the ratio of actual power emitted to the power emitted by a black-body radiator. As such, an emitting source following a black-body emission model will have a constant emissivity of one, $\varepsilon = 1$. So called grey emitters in the plume, such as large aluminum agglomerates and alumina soot particles, will have constant emissivities that are less than one as black-body radiation represents an ideal emission model. Three emissivity models are considered in this work: 1) black-body emission, 2) $1/\lambda$ wavelength dependent emissions, and 3) $1/\lambda^2$ wavelength dependent emissions. The difference between grey and black-body emissions is expected to be relatively small and, as such, a black-body emission model is used. When the size of an emitting body is on the order of the wavelength of light being emitted it is possible for the emissivity to become wavelength dependent, $\varepsilon=\varepsilon(\lambda)$, when the classical Lorentz oscillator model is considered (6). Specifically $\varepsilon(\lambda)=1/\lambda$ and $\varepsilon(\lambda)=1/\lambda^2$ emissivity models are used where $1/\lambda$ dependency may be caused by molten aluminum agglomerates and $1/\lambda^2$ may be caused by the presence of micron sized or smaller aluminum and alumina particles [7] [8]. Wien’s displacement law may also be developed using wavelength dependent emission models through the use of poly-logarithm functions [9] as given below

$$\lambda_{\text{max}} T = \frac{hc}{k_B} \frac{1}{5 + W_0(-5e^{-5})} = 2.898 \times 10^6 \text{nmK}$$

(1)

Where $h$ is Planck’s constant, $k_B$ is Boltzmann’s constant, $c$ is the speed of light, and $W_0$ is the Lambert function. For sufficiently small arguments the Lambert function may be approximated by its argument, $W_0(x) = x$, and leads to the Wien approximation. When using $1/\lambda$ and $1/\lambda^2$ emission models, the resulting temperatures show a 5/6 and 5/7 reduction as shown below.
for $1/\lambda$ dependence and

$$\lambda_{\text{max}} T = \frac{hc}{k_B} \left(\frac{1}{6 + W_0(-6e^{-6})}\right) = 2.415 \times 10^6 \text{nmK}$$

(2)

for $1/\lambda^2$ dependence. To further illustrate this effect, consider a black-body emitter with a maximum wavelength emission of 1000nm which has a corresponding emission temperature of 2898K. Wavelength dependent emissivity models will have temperatures of 2415K and 2070K for $1/\lambda$ and $1/\lambda^2$ emissions, respectively.

The maximum wavelength emission for the spectra observed from the propellant is expected to be in the 1000-1300nm range. Given the decreased sensitivity in the nominal 1000nm wavelength region, the limited range of the instrument and the expected temperatures from propellant plume direct peak fitting with Wien's Displacement law is not preferred for determining the flame temperature. Rather fitting with a semi-log approximation of the Planck equation is performed [7, 8] where the approximation is given by

$$\ln \left(C \ast \frac{I(\lambda, T) \ast \lambda^5}{\varepsilon(\lambda)} \right) = -\ln \left(\exp \left[\frac{hc}{k_B \lambda T} \frac{1}{\lambda^5} \right] - 1 \right) \approx -\frac{hc}{k_B} \frac{1}{\lambda T}$$

(4)

where $C$ is a constant, $I(\lambda, T)$ is the recorded spectrometer intensity, and $\varepsilon(\lambda)$ is the emissivity model. Using this fitting method the natural logarithm of the collected data multiplied by $\lambda^5$, $\lambda^6$, and $\lambda^7$ for constant, $1/\lambda$, and $1/\lambda^2$ emissivity models are plotted against the inverse wavelength and are fit using linear least squares methods. The slope of the fitted line is used to determine the temperature by way of the approximation in equation 4. A typical fit of this kind is shown in Figure 4 which corresponds to the same propellant burn shown in Figure 3 for AlO emissions. Contributions from atomic and molecular spectral emissions have been removed to reduce the error of the fit. Such emissions are AlO, sodium, potassium, aluminum, and iron. The inferred temperatures in Figure 4 are $2472 \pm 84K$, $2208 \pm 74K$, and $1991 \pm 67K$ for constant, $1/\lambda$, and $1/\lambda^2$ emissions, respectively. The errors are inferred from the systematic error in the slope associated with the linear least squares fitting and also include a three percent error that accounts for the approximation. Typical temperatures from a downward burning propellant are found to be in the nominal 2200-2500K range with typical errors falling into the 65-80K range.

5. Carbon dioxide and water gases

Gas (CO$_2$ and H$_2$O) and broadband radiation were measured using two ES100 Spectraline spectrometers from En’Urga Inc. They were placed orthogonal to each other with the propellant burn at the center of view of both spectrometers; see Figure 5. This setup allows emission tomography measurements in multiple angles of the propellant exhaust. The two spectrometers measured in a band of 1.3 to 4.8$\mu$m, sampling 256 wavelengths with 0.018 $\mu$m resolution. Each spectrometer scans 128 angles at a rate of 1.32KHz for full 128 angles measurement at 10.3Hz. The use and placement of two spectrometers is intended to determine the transmissivity distribution around the propellant.

Temperatures at each angle are calculated by looking at local spectral radiation intensity measurement, where the spectral specific emission coefficient, $a(\lambda)_{nm}$ for that path is calculated for each homogeneous region using a radiative transfer equation [10,11].

$$I(\lambda)_n = \sum I(\lambda)_{Bnm} \ast \left(1 - e^{-k(\lambda)_{nm}\Delta_{nm}}\right) = \sum I(\lambda)_{Bnm}a(\lambda)_{nm}$$

(5)

Where n is the angle being analysed, and m is the region where the blackbody temperature and plume transmissivity are quasi-homogeneous. $k(\lambda)_{nm}$ is the spectral specific emission coefficient for the angle n, and exhaust region m. $\Delta_{nm}$ is the path length in that region. All 128 equations are then linearized:
where

$$\log(I(\lambda)_n) \approx \log(I(\lambda)_{BBm}) + \log(1 - \tau(\lambda)_{nm}), \quad \text{Where } \alpha(\lambda)_{nm} = 1 - \tau(\lambda)_{nm} \quad (6)$$

Figure 5. Setup for measuring CO$_2$ and H$_2$O gas molecules. Two orthogonal spectrometers with 128 scanned angles each. Each spectrometer measures from 1.3 to 4.8μm at a rate of 1.32KHz with a full spectra set (all angles) at a rate of 10.3Hz.

The equation is set up to solve for two linear equations:

$$\log(I(\lambda)_{BBm}) \approx C_0 \lambda m + C_1 m T_m \quad (7)$$

$$\log(1 - \tau(\lambda)_{nm}) \approx C_2 m + C_3 \lambda X(\lambda)_{CO_2m} + C_4 m X(\lambda)_{H_2O m} + C_5 m T_m + C_6 m f_m \quad (8)$$

Equation (5) can be written:

$$\log(I(\lambda)_{n}) \approx C_0 \lambda m + C_2 m + C_3 \lambda X(\lambda)_{CO_2m} + C_4 m X(\lambda)_{H_2O m} + (C_1 m + C_5 m) T_m + C_6 m f_m \quad (9)$$

Where C3, C4 and C6 are larger than zero, C1+C5 > 0, \(\log(I(\lambda)_{BBm})\)-C0-C2 > 0 and all the constants are non-negative. \(X(\lambda)_{H_2O m}\), \(X(\lambda)_{CO_2m}\) are the volume fractions for H$_2$O and CO$_2$ respectively, and \(f_m\) is the volume fraction for soot [12,13]. C2, C3, C4, C5 and C6 are found in the RADCAL database [14]. The linear equations require at least six wavelength measurements, and it can be solved by the maximum likelihood estimate (MLE) method [15]. The algorithms guess the transmittance of the regions in the propellant, in this case rings, and use the MLE to calculate the local intensities, which recalculate the local transmittances until the algorithm converges.

Figure 6 shows an intensity distribution obtained from one ES100 Spectraline units. The surface distribution is a function of angle and wavelength, showing the spectral locations of CO$_2$ and H$_2$O from an upward burn test. This measurement is a snapshot during the steady burning. Figure 7(a) shows the setup for a downward setup and the location of the spectrometers with respect to the propellant, a substrate (in this case a graphite plate) and the plume. The diagram is not to scale and the propellant...
to substrate gap starts at 50.8mm, and increases as the propellant is consumed. The line of sight of the spectrometers was set at 50.8mm from the substrate. Figure 7(b) is the instant measured temperatures for the two gases and the soot. The propellant diameter in this test was 508mm in diameter. Gas temperatures were greater than 2500K, and soot temperatures were approximate 1800K.

![Figure 7](image)

**Figure 7.** (a) Downward burn basic schematic with propellant 50.8mm above graphite plate (b) Temperature measurement for gases and particles for a downward burn; the abscissa is the radius from the center of the propellant.

### 6. Hydrogen chloride gas

Hydrogen chloride (HCl) gas is one of the byproducts of burning aluminum and ammonium perchlorate, the main ingredients in some solid propellants. HCl is a diatomic molecule with emission spectra in the mid-wave infrared (2μm - 5μm) showing a rotational-vibrational spectrum centered at $\lambda_0 = 3.4598\mu m$ (2890.34cm$^{-1}$). This wavelength is the transition from ground state to the first excited vibrational state. There is not emission at this wavelength, see Figure 8, but rotational emission lines are seen at both sides of that wavelength following a Boltzmann distribution.

![Figure 8](image)

**Figure 8.** Measured HCl spectrum at the mid-wave infrared. Notice the P and R Branches with the rotation-vibrational emissions with an envelope following a Boltzmann equation. The shape and location of the peak of the envelope is determined by the temperature of the gas.

The measurements of HCl were performed with a Nexus 670 Fourier transform infrared (FTIR) spectrometer. An FTIR is a modified Michelson interferometer; see Figure 9, which has a moving mirror in one of its arms. Every scan of the mirror generates an interferogram that will be Fourier
transformed to generate a spectrum. The length of the scan is inversely proportional to the resolution of the spectrum measured. This means that for higher resolution measurements the mirror will take longer to conduct a scan. A 1 cm\(^{-1}\) measurement typically takes 3 seconds, and a 0.25 cm\(^{-1}\) measurement will take approximately 12 seconds, if there are no large changes in the light flux. Otherwise, the auto-gain step can add 4 more seconds. The 1 cm\(^{-1}\) resolution was selected because it balances the requirement for high speed measurement and the ability to resolve the HCl lines.

![Figure 9. FTIR basic spectrometer schematic with light collecting optics.](image)

The instrument was used in single beam mode without a reference blackbody source. Light from the propellant was gathered though an external port. The spectral response of the system is delimited by the liquid nitrogen cooled mercury cadmium telluride (MCT) detector (2-5 μm). Light from the propellant was collected using two 76.2 mm off-axis parabolic mirrors. The one in front (objective mirror) was the main gathering optical components. The light was focused into an iris where it was spatially filtered and then a second off-axis parabolic mirror collimated the light into the FTIR. There were cases were the pin hole was not used, but the gathered light was considered collimated when it was coming through a 1016 mm long alumina tube. The collecting optics and the FTIR were always aligned at the center of the gap between propellant and substrate. For experiments where the gap was 12.7 mm or less, the data were extremely noisy and no spectrum fit could reach \(r^2 > 0.9\), making the data unusable. This was later overcome with experiments using the 1016 mm long alumina tube. The alumina tube was used to avoid the soot and dust from the propellant exhaust.

![Figure 10. HCl P-branch spectrum showing the fine structure of the vibrational rotational emission.](image)

Most of the preliminary analysis on the HCl was done on the P-branch. From a careful look at the spectrum of the P-branch, it is possible to see the emission peaks from Cl\(_{35}\) and Cl\(_{37}\). The R-Branch
seems to overlap with the water emission spectra. There are some water emission lines in the P-branch that reach 3.5μm, but they do not overlay with the HCl lines, see Figure 10. However, the P-branch shows a higher than normal emission line around 3.771μm. Some modeling is underway to verify that this line is a rotational-vibrational emission from nearby vibrational excitation and the line is close but does not overlap the line in 3.771μm. The FTIR is, at this instance, unable to resolve that extra line on high resolution measurements (0.25 cm$^{-1}$).

Temperatures were calculated by a modified version of the method used by Zhang et al. [16], and Herzberg [17]. An equality relates the spectral running number, m, of each line in the P and R-branches to a linearized Boltzmann distribution:

$$\ln \left( \left| m \right|^4 \right) = \frac{B \cdot \hbar \cdot c}{k \cdot T} \cdot m(m+1) + b$$

(10)

for integer $m= 1, 2, 3,..$. From measured spectra, the frequency of each peak is elevated to the power of four, $\nu^4$, multiplied by the magnitude of the running number, $|m|$, and divided by the line corresponding peak. The right side of the equality is the linearized form of the Boltzmann distribution multiplied by the rotational constant $^7$, $B_c = 10.5934$ cm$^{-1}$, times the running number $m(m+1)$, where c is the speed of light, k is the Boltzmann constant, T is the temperature, and h is the Planck constant. Plotting the right side of equation 10, versus the $m(m+1)$ relationship, provides a series of points that can be fit to a straight line, see Figure 11.

The slope, A, of the line is equated to the linearized Boltzmann distribution, from which the temperature of the gas is calculated:

$$T = \frac{B \cdot \hbar \cdot c}{k \cdot A}$$

(11)

Figure 11. The linearizing of peaks for the fine emission spectra of the P-Branch can be fit to a line and its slope used to calculate the temperature of HCl. A more sophisticated code uses the P & R branches.

Preliminary work focused on the P-branch because it is the less noisy of the two branches. The calculated temperatures were high, usually in the order of 3000K. These numbers are hard to dismiss as previous measurements showed similar temperatures. The numbers from the R-branch were extremely low, on the order of 1200K to 1500K, and are suspect because the R-branch straight line fits tended to be lower than the fits from the P-branch. Further analysis was done using temperature measurements from both branches and correlated to laboratory measurements of HCl emissions inside an oven. The set temperatures of these tests ranged between 963K and 1863K, for a total of 10 temperatures, with equal 100K steps. The measurements showed that the calculated temperatures could be 600K higher than the oven temperature settings when using only the P-Branch. The error reduces to 100K when using the average temperature from both P and R-branch. If we use both

$^7$ NIST: http://ccdb.nist.gov/exp2.asp?casno=7647010
branches in the calculation for all propellant tests, then the average temperature is 2247K with an error of +360K/-270K. These numbers are restricted to measurements with line fits, $r^2$, greater than 0.9.

7. Conclusions
This paper presents the complex conditions for off-design solid propellant tests, where multiple gases, aluminium monoxide and soot provide different temperatures and conditions that can mask the effects of each other. Three spectral measurement methods were presented, each looking at a different species (AlO, HCl, H$_2$O, and CO$_2$). Each method is in a different state of development. Where the spectral tomography measurement of H$_2$O and CO$_2$ has had years of refinement, the work on FTIR measurement of HCl is still in the initial stages, and will require refinements to eliminate a 100K difference between the test oven reported temperatures and the spectrally calculated ones. Understanding the different temperatures with respect to the different species should provide a better picture of what an RTG will be exposed to in an accident scenario.

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