
***A Compact Borehole, Thermal-Infrared
Radiometer and Infrared Reflectometer for the
Characterization of Subsurface Habitability
and Presence of Water Ice on Mars***

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A THESIS SUBMITTED FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY

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July 2016

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Abstract

One of the most important steps in the search for life on Mars is to determine if a specific sub-surface location it is “habitable”, or that it provides the conditions and requirements to support life as we know it. In this thesis, I present a miniature, thermal-IR radiometer and reflectometer designed to determine temperature, the presence of water ice, and the discrimination of minerals, all necessary for a habitable environment.

A dual use detector was selected for the thermal and five reflectance channels. The IR source is provided by five LEDs. These components were embedded in a thermally controlled aluminium block. Integrated electronics provided signal amplification and demodulation. This device will be suitable for drilling applications with less than 25 mm diameter boreholes and with limited available power (<5watts).

Thermal testing was within a simulated borehole mounted in a thermal vacuum chamber. The results were compared to a theoretical model of the expected temperature. The maximum temperature error between predicted and measured was 0.21 K (~0.08%). The total RMS error of all sources were calculated to be <3%.

Reflectance testing in all five channels included a variety of minerals and a two point calibration method. The results were compared to the predicted reflectance values for the samples. The results of the reflectance channel testing demonstrated that the measured values matched the predicted values with a 2.5% measured error. The total RMS error was 6.1%.

Detection and discrimination of water ice and hydrated minerals included a non-linear mixing model and/or testing. The model predicted that water ice mixed in a pyroxene mineral matrix can be detected and discriminated from 5% to 60% concentration by weight. Testing with a hydrated mineral mixed within a non-hydrated mineral matrix demonstrated that the measured result matched the predicted result from 5-45% concentration by weight.

Acknowledgements

The development of any doctoral thesis relies on the help of many people and who have my eternal gratitude. The encouragement of my many friends was central to pushing through the many difficult moments. Matthew Ritchie, Susan Graham, and Irina Fedorenko who constantly had my back and gave me the time I needed to complete this thesis. Mr. Wilf Stephenson, the Middle Common Room (all six years!), and the entire staff at Oriel College for providing a pleasant place to live for 5 years and much patience when funding got tight. My family for their numerous contributions. My father for his constant and inspirational interest in science and technology and who made me promise to take at least one physics class at the university. A kept (and well-exceeded!) promise that has opened more doors than I could have ever imagined. Generous financial support from my father, my great-grandmother, and Uncle Sam provided me the flexibility to pursue all of my crazy dreams. And especially, my mother whose door was always open when I needed it most.

I would like to thank the following people for their time, comments, and support. Dr. Gian Gabriele Ori for organizing the Field Expeditions to Morocco and the Rio Tinto and the many great field researchers on these trips who helped in the identification and selection of the analog materials collected for this thesis. Dr. Julio Valdivia-Silva and Saul Perez-Montaña, who have been steadfast collaborators and friends for more than a decade in Peru and whose contributions to this project are too numerous to list. Dr. Charles Cockell for his insights into Astrobiology fieldwork. Dr. Owen Green of the Earth Sciences Department for help and access to the equipment necessary for processing analog materials. Ian Thomas for help in the initial spectral analysis. Takahiro Hiroi from Brown University RELAB for the full spectral characterization of all collected samples. Tristram Warren and Shuning Bian for their help with the electronics design and testing. Shuning Bian for his help in writing the Arduino control code. Jon Temple, Andy Clack, and Gregory King in the AOPP electronics lab, and the technicians in the physics mechanical shop for their technical support building my instrumentation. Josh Emery for providing his Hapke Model IDL widget. Josh Emery and Ted Roush for providing most of the

optical constants. Dr. Simon Calcutt for providing additional financial support for thesis supplies. The final step is the public examination, and I would to thank my External Examiner, Dr. Peter Grindrod, and Internal Examiner, Professor Fred Taylor, for agreeing to and taking the time to read my Dissertation and to challenge my assumptions and choices. It was an amazing conversation! Thank you!

As always, Dr. Christopher McKay for his support financially (under the NASA ASTEP Program, Grant NNX11AG33A), in the development of the scientific background, and for his encouragement (*“Lauren, remember the most important thing to get out of graduate school.....yourself!”*).

And, most importantly, my graduate program supervisor, Dr. Neil Bowles, for his constant availability and willingness to help “A Nevada Yankee in King Arthurs Court.”

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Chapter 1: Introduction

1.1 Introduction to the project

Humankind has long had a fascination with the search for life beyond the Earth and, in particular, on Mars. The idea that planets might be habitable and full of life is practically as old as the concept of a planetary body. “Cosmic Pluralism” or the idea that life might be seeded throughout the cosmos, is generally attributed to the Greek philosopher and astronomer, Thales (c. 624 BCE – c. 546 BCE) (Brake, 2006). One of the earliest works on the subject of the life of Mars is *Cosmotheoros* written by Christiaan Huygens and published posthumously in 1698. Huygens discusses what is required for a planet to be capable of supporting life, speculates about intelligent extra-terrestrials, and suggests for the first time that, even though Mars will be colder than Earth, life there will have adapted (Karol and Catling, 2009).

Central to the understanding of if and how life might have developed on Mars, is the determination of the habitability of any specific location. Past and future results in the search for life on Mars can only be correctly interpreted with information regarding the habitability of a specific environment (Klein, 1978, Stoker et al., 2010).

The modern exploration of Mars started with the U. S. led Mariner 9 orbiter in 1972 that took the first photographs of topological evidence of past water flowing across the surface. There have been 21 successful missions to Mars. Some of the most important results, and their importance to this thesis, are related to finding water (in either the past or in current conditions) which is considered the key to life (McKay, 1998). The evidence for water in the past and the existence of frozen and liquid water on present day Mars is extensive (Grotzinger et al., 2014, Heldmann et al., 2010, Malin et al., 2006, McEwen et al., 2011, Renno and Mehta, 2010, Smith et al., 2009), yet no life (present or extinct) has been found to date. It is likely that the current surface environment is too hostile to even bacterial forms of life, and it would appear that sub-surface environments are the best hope for finding extant life on Mars (McKay, 1997). Therefore, the hypothesis of this thesis is, **“The subsurface environment of Mars provides habitable conditions sufficient to support life.”**

New missions to Mars are under development, many of which have a drilling component with the purpose to better understand the subsurface environment. While new sensors and technologies are being developed expressly for these types of drilling missions (Table 1-5), there is a lack of options that are compact enough to meet the size and power limitations of borehole instrumentation, especially in terms of the search for life and determination of habitability in the subsurface.

This thesis was funded in large part by a NASA grant titled, “Icebite” (P.I.: Christopher McKay). The Icebite project was for the development of an ice-coring drill-bit device (Section 1.3). This thesis was funded to create an instrument to detect and discriminate water ice percentages in a sub-surface soil matrix; however, as part of the academic program, was expanded to address habitability in sub-surface environments.

The two fundamental concepts of “life” and “habitable environment” are complex, but can be reduced to a simplified set of “requirements for life” (in the broadest sense). These, in lieu of a definition of life, allows us to think about conditions on any planetary body that would satisfy these requirements. For the purposes of this thesis, “habitable” will be defined as *an environment that provides a source of energy, a liquid solvent, and raw materials under conditions sufficient to support life* (Hoehler et al., 2007, Hoehler and Westall, 2010, Stoker, 2008).

These still can lead to a complex set of conditions to measure, so two guiding strategies are suggested in order to arrive at a first order approximation of a habitable environment. These are “follow the water” and “follow the energy.” Since water is the most likely liquid solvent on Mars, the search for life begins with finding a source of water (in either liquid or solid form). This is closely followed by the determination of a viable source of energy. Because the hypothesis of this thesis limits the search to subsurface environments, only chemical sources of energy are considered. These are the exothermic oxidation-reduction of minerals in the natural environment which provide energy (Gibbs free energy, $\Delta G^\circ > 0$, typical) necessary for cellular biosynthesis.

An in-depth analysis of what constitutes a habitable environment (Fletcher et al., Submitted) led to a series of specific questions (Table 1-1). Each of the questions are directly related to the discovery of water, a viable source of energy, materials necessary for building

cellular mass, and the state of the environment over time. The answers to these could be used to quantify the habitability of subsurface environments on Mars in all of its epochs. Past refers to warm and wet Mars, Present refers to cold-dry Mars up to the present time, and Episodic refers to periods of time when the surface conditions are sufficient to produce liquid water. These are used as additional guidance for instrument selection, design, and testing throughout the rest of the project.

Table 1-1: Science questions for subsurface habitability

Cat.	Question	Epoch of Habitability		
		Past	Present	Episodic
I	What is the subsurface temperature?		X	X
I	Is there water trapped in the rocks?		X	X
I	Is there permafrost?			X
I	Can we determine salinity?		X	X
I	Are there aqueous altered materials?	X		
I	What is the stratigraphy?	X	X	X
I	Are there salts (gypsum, halite or other)?		X	X
II	Is there a chemical energy source?	X	X	X
III	Are there the raw materials?	X	X	X
IV	Can we detect organisms?	X	X	X

Category: I – Water; II – Energy; III – Raw Materials; IV – Direct Detection of Life

1.2 Science objectives as measurable physical properties

The scientific questions presented in Table 1-1 can be translated into measurable scientific objectives designed to answer the questions. Each of these is discussed in detail in the following paragraphs. These are:

- Material surface temperature
- Presence of bonded water and water ice
- Water ice percentage
- Presence of hydrated minerals
- Detailed mineral discrimination (as a thesis goal)

Temperature

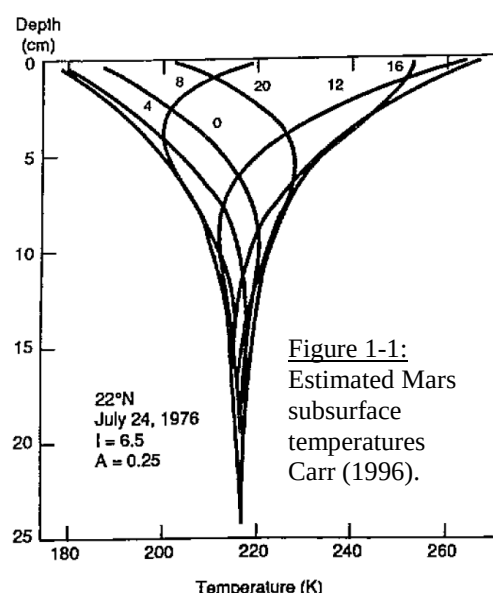
The required temperature range was based on three intended locations of operation. These are: 1) the Atacama Desert, Peru, 2) University Valley, Antarctica, and 3) Mid-latitudes, Mars. Actual surface temperature ranges of the three environments are provided in Table 1-2.

Table 1-2: Range of Environmental Parameters in Analog Environments and on Mars

Environment	Surface Temperature Range*, K (°C)	References
Atacama Desert (Yungay):	267 to 323 (-6 to 50)	(Davis et al., 2010, McKay et al., 2003, Warren-Rhodes et al., 2006)
Antarctic Dry Valleys (Linneaus Terrace):	231 to 269 (-42 to -4)	McKay et al. (2009, 1998)
Mars: Mid-Latitudes Mars at Depth (@15 cm)	183 to 298 (-90 to 25) 213 to 218 (-60 to -55)	(Carr, 1996, McKay et al., 1998, McKay et al., 2009)

*Note: These are typical ranges, and these values can be exceeded on rare occasions.

While the surface temperatures of Mars can vary significantly from diurnal to nocturnal, the temperatures stabilize by 25 cm of depth in the subsurface as shown in Figure 1-1 (Carr, 1996). From an analysis of the environmental parameters, a measurement range of 190K to 330K is proposed. Testing will be bounded by low temperatures in Antarctica and high temperatures in the Atacama (230K to 323K).



Water ice and percentage

The capability to detect the presence of water ice is a priority in the development of the instrument. This measurement is a simple positive or negative detection requirement; however, in a subsurface soil environment, the percentage content can vary according to the local environmental conditions. In the case of the Atacama, it is expected that there will be no measureable water content beyond a variation in subsurface relative humidity (RH) between diurnal (low RH) and nocturnal (high RH) periods (McKay et al., 2003). The quantity of water

ice in subsurface environments in both the Antarctic Dry Valleys and on Mars can vary. In terms of Mars mid-latitudes, percent weight (wt %) of water ice in soils was determined to vary from 1 to 15 wt % (Milliken et al., 2007). The evapo-transpiration rate mechanism in University Valley, Antarctica, is similar to Mars and water ice varies from 1 to 15 wt % (Levy et al., 2011). This is used as the required measurement range for the determination of wt % water ice.

Hydrated minerals

For this thesis, hydrated will include minerals with bonded water and/or hydroxide (OH⁻), though the latter are technically hydroxylated minerals. The distribution of hydrated minerals is important to understand in order to determine the geological development of Mars and for the determination of the habitability of the planet's past and present. As a minimum, the detection (positive or negative) of hydrated materials is required. Categories of hydrated materials are provided in Table 1-3.

Table 1-3: Categories¹ of Aqueously Altered Materials

Category	Representative Materials	Mineral Selected	Chemical Formula ²	Mars Reference
Ferric oxo-hydroxides	Hematite, goethite	Hematite	Fe ₂ O ₃	Christensen et al. (2001b)
Carbonates	Calcite, siderite, magnesite	Calcite (Ca-carbonate)	CaCO ₃	Morris et al. (2010), Ehlmann et al., (2008)
Fe-sulphates	Jarosite, halotrisite, alunite	Jarosite	KFe ₃ (SO ₄) ₂ (OH) ₆	Golden et al. (2008)
Sulphates	Barite, gypsum	Gypsum	CaSO ₄ ·2H ₂ O	Gendrin (2005), Bridges & Grady (1999), Rieder (2004)
Phyllosilicates	Al- phyllosilicates, Fe/Mg smectites, montmorillonite, serpentine	Montmorillonite serpentine	(Na,Ca) _{0.33} (Al,Mg) ₂ Si ₄ O ₁₀ (OH) ₂ ·nH ₂ O Mg ₃ Si ₂ O ₅ (OH) ₄	Bishop(1993), Bibring et al., (2005), Poulet al., (2005)

Notes: 1) Table modified from Valdivia (2008), 2) Duda and Rjl (1998).

Table 1-3 shows a reduced set of general categories of materials as well as representative minerals that fall under that category, and the specific mineral that has been selected to represent that category for the purposes of this thesis (Thollot et al., 2012, Valdivia-Silva, 2008). Two additional categories of aqueous altered materials include chlorides and opaline silica; however, these are not considered for this thesis due to low concentrations on the surface. The presence of

these materials provides an indication of past water on Mars, but they also provide the energy source and/or elements needed for microbial growth. All of the selected minerals have been found on the surface of Mars as referenced in Table 1-3. Analogue samples of these materials were collected from locations around the Earth and are described in detail in Chapter 2 (Table 2-2).

Mineral discrimination

The discrimination of hydrated mineral categories (Table 1-3) mixed with non-hydrated minerals is highly desired as an overall goal of this project. For this thesis, discrimination will be limited to the determination of the percent distribution of minerals. This will be balanced by time and cost of materials necessary to build this additional capability.

Science requirements summarized

Table 1-4 provides a list of the science objectives and the measurement requirements. These form the basis for the selection of materials and technologies, development of the theoretical models, and pilot bench-top testing in the following chapters.

Table 1-4: Science Objective Requirements

Science Objective	Requirement
Temperature –Full Range:	190K to 330K
In practice:	230K to 323K
Water Ice	Positive or Negative
Water Ice Percentage (by weight)	1 to 15%
Hydrated Minerals	Positive or Negative
Mineral Discrimination	Thesis goal

1.3 Additional limitations applied to drilling missions

The goal of this instrument is investigating the habitability in the subsurface of Mars within a small diameter (<30 mm) borehole using compact *in situ* sensors. This will provide science return in three ways, 1) Details of the borehole will be revealed, 2) Provides context for the detailed analysis of samples by surface instruments, and 3) Provides the opportunity for real-time, strategic decision making for surface instrument teams.

Per the direction of the NASA technical monitor for this project, it was decided early on to focus on the functionality of the sensor system development as independent of any drilling operations (McKay, personal communication, May, 2011). For this reason, the implementation design concept is for a post-drilling borehole probe and will not be integrated into a drill-string.

Additional criteria included limiting the choice of a detector to uncooled and no moving parts. There was no time or budget for custom components design and manufacturing, so a technology demonstration prototype was limited to commercially available components (designated as Commercial Off the Shelf Components (COTS)). Finally, components with flight heritage were preferred.

1.4 Methods and technology for measurement of science objectives

There are a number of approaches for the measurement of the science objectives (Table 1-4) that have been used on Earth and during previous Mars missions (Botta et al., 2008). These include physical, chemical/biochemical, analytical, and contactless. Physical can include direct contact sensors to measure the surface temperature, salinity of a solution, and mass-loss methods of the determination of water content via evaporation. Chemical/biochemical can include liquid chemistry methods for the extraction of carbon, nitrogen, minerals, and bio-molecules. Analytical can include the use of Gas-Chromatograph Mass Spectroscopy (GC-MS) to determine mineral content and distribution; Atomic Absorption for the determination of elements; or High Power Liquid Chromatography (HPLC) and Pyrolysis-GC-MS for the determination of organic molecules. Contactless methods include infrared emission and reflectance for the measurement of temperature and the measurement of spectral properties to determine mineral content using spectrometers, radiometers, and lasers.

Previous solutions for Mars exploration

Previous lander and rover missions to Mars have literally only scratched the surface. At most, missions such as Viking 1 & 2, Phoenix, and Curiosity have used scrapers, shovels, grinders, and drills to collect samples from no more than 5 cm of depth; however, there are a number of instruments in development for subsurface analysis as noted in Table 1-5.

These new types of instruments can be categorized into three general types:

- I. Borehole sample extraction for surface based instrument: Planetary Underground tool (PLUTO) (Richter et al., 2003), IceBite (McKay et al., 2008), Mars Astrobiology Research and Technology Experiment (MARTE) (Cannon et al., 2007), ExoMars (De Sanctis et al., 2014).

- II. Moles; One way design, either borehole or full mole: Vanguard (Ellery et al., 2005), Heat flow and Physical Properties Package (HP³) (Spohn et al., 2012), and Water Sensor (WatSen) (Grady, 2006, Wolters et al., 2013).
- III. In situ borehole instrumentation:
- Fully integrated borehole instrument: Laser-induced breakdown spectroscopy (LIBS) (Moreschini et al., 2011), APXS (Kelliher et al., 2008), Mini BSL (Bramall et al., 2006), Neutron Probe (Elphic et al., 2006), Raman (Cannon et al., 2007), Visible Cameras (Cannon et al., 2007).
 - Sensor head mounted in borehole probe with fibre optic cable running up to surface based instruments: Ma_Miss (De Sanctis et al., 2014), Vanguard (Ellery et al., 2005), and IR/Raman Spectrometer (IOSPEC) (Jessen et al., 2007).

Table 1-5: Types of Borehole and Mole Instruments for Mars Subsurface Exploration

Instrument	Lander	Rover	Mole	Mission	Retractable	In Situ Borehole Activity
Ma_Miss		X		ExoMars	X	Borehole Sample Extraction Borehole Instrument: Sensor head with fibre optics cable to surface instruments for mass spectrometry
PLUTO	X			Beagle 2	X	Borehole Sample Extraction
IceBite	X			Future	X	Borehole Sample Extraction
MARTE	X	X		Future	X	Borehole Sample Extraction Borehole Instrument: Raman Spectrometer, Visible Cameras
Mini BSL	X			Future	X	Borehole Instrument: Bacteria Detector
Borehole Neutron Probe		X		Future	X	Borehole Instrument: Ice Detection
APXS	X	X		Future	X	Borehole Instrument: X-Ray Spectrometer
IOSPEC		X		Future	X	Borehole Instrument: Sensor head for spectrometer, Surface based Raman Spectrometer, IR Spectrometer
LIBS (Honeybee)		X		Future	X	Borehole Instrument: Laser Induced Breakdown Spectroscopy (LIBS)
Vanguard			X	Future	-	Mole Type Borehole Instrument: Sensor head for spectrometer, Surface based Raman Spectrometer, IR Spectrometer, Mass Spectrometer
HP ³			X	Insight	-	Mole Instrument: Heat flow, Thermal Conductivity
WatSen			X	Future	-	Mole Instrument: RH, IR Spectrometer

Each of these has advantages and disadvantages as presented in Table 1-6. While the science requirements drive the selection of the instrumentation, this is often tempered by the operational limitations (power, mass, size, etc.). The goal in the selection of instrumentation is to balance getting the most of the science requirements while in a highly optimized design. Compromises are always made, but have to be carefully considered and justified.

Table 1-6: Comparison of mission types and configurations

Mission Type	Configuration	Advantages	Disadvantages
Sample Extraction for Surface Based Instruments	Full Bore Core: MARTE	• Full core analysis by surface instruments • Full borehole analysis by borehole instruments • Allows cross-correlation of full borehole stratigraphy to core sections • Allows full analysis by instrumentation that cannot be packaged for a down-hole instrument	• Significant additional structure, mass, power • Same for full borehole core • Lander mission only • Single use device
	Mini-tip core: IceBite, PLUTO	• Small diameter drill string (less energy, weight, etc.) • Not a full length core • Can take several samples throughout the borehole • Can be used on larger rovers • Allows full analysis by instrumentation that cannot be packaged for a down-hole device	• Blind-point measurements • Borehole stratigraphy and sample context lost with point measurements • Lander mission only • Single use device
<i>In situ</i> Mole Instrumentation	Fully integrated Instruments: HP ³ , WatSen	• No Borehole to navigate • Low Signal to Noise Ratio (SNR) or spectral attenuation through Fibre Optics • <i>In situ</i> measurement • Context not lost with removal of sample from borehole	• One-way trip • Single use instrument • Not possible to combine mole data with data from extracted samples with surface instrumentation
<i>In situ</i> Borehole Instrumentation	Single use Mole; sensor head and fibre optics cable to surface based instruments:	• <i>In situ</i> measurement • Context not lost with removal of sample from borehole	• One-way trip • Limited number of borehole moles available (3 for Vanguard) • SNR transmission losses through fibre optic cable
	Retractable; sensor head in borehole and fibre optics to surface based instrument:	• <i>In situ</i> measurement • Context not lost with removal of sample from borehole	• SNR losses or spectral attenuation through fibre optic cable

Lessons learned from previous missions

There are lessons that can be learned from an analysis of these designs. These can be applied to selection of specific technology and methods to meet the science requirements of this project.

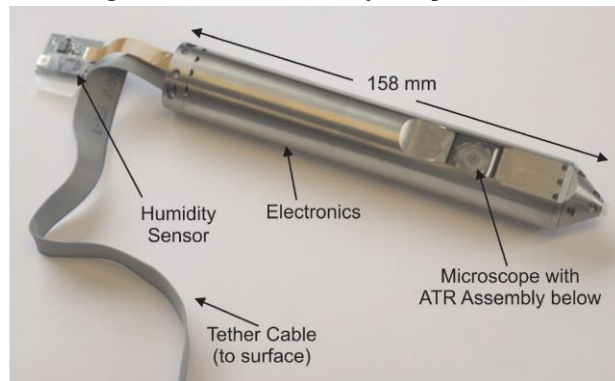
- I. Borehole specific data are essential to provide context for the interpretation of results of samples removed for analysis by surface instruments.

- II. Small borehole diameters limit/eliminate some instrumentation from *in situ* borehole applications.
- III. Reduced capability for *in situ* measurements to allow for a comparison to surface measurements is preferred to no data.
- IV. *In situ* sensors & analysis in borehole is preferred to potential limits to the wavelength range associated with fibre optics spectral absorption properties.

WatSen as an example of a subsurface instrument

One of the best examples of a compact subsurface instrument is the WatSen instrument which was developed for the European Space Agency under contract to the Open University (UK), DLR (Germany), and Norsk Elektro

Figure 1-2: Watsen and key components



Optikk (Norway) (Wolters et al., 2013). This is a compact device designed for use with a mole (such as HP³) and includes an attenuated total reflectance (ATR) mid-IR spectrometer, microscope, humidity sensor, and surface contact temperature sensor. It has a diameter of 26 mm and power consumption of <3 watts (Figure 1-2). The main objective is to detect water absorbed on the surface of soil grains while the secondary goals are to determine the mineralogy, mineral chemistry, and grain size, morphology and porosity of the soils with depth. The ATR spectrometer includes a thermal infrared source, diamond ATR crystal, and pyroelectric sensor array. The spectral range is 6.2 to 10.3 μm with a 40 nm resolution to allow for the detection of water (combined with data from the humidity sensor), while still being able to distinguish the principal components of the basalt surface material (pyroxene, olivine, and plagioclase), and to identify carbonates. The surface-contact, temperature sensors allow heat-flow experiments.

WatSen has very similar requirements to those required for this project. This approach has some good points in that it is a full spectrum spectrometer with moderate resolution. The mid-IR range allows a good discrimination of the required minerals and detection of water (especially when the spectral data are considered in context of the RH sensor). The ATR requires that the diamond window be in direct contact with the sample grains. Because this was designed to be

used with the HP³ mole, this works well; however, a retractable borehole device may have difficulties utilizing this approach as it is expected to be a contactless device.

Contactless methods as the preferred approach for borehole instrumentation

Due to the constraints of the borehole diameter and power limitation, the use of physical methods with retrieved samples, liquids, and bulky analytical methods are not possible. This leaves contactless methods as the best option that will allow the measurement of the science objectives while meeting the physical constraints of a retractable, borehole instrument.

1.5 Review and selection of methods and technology for this project

Many materials have spectral characteristics (e.g., absorption bands) which can be determined from IR reflectance and thermal IR emission measurements (Anderson et al., 2005). These IR spectral characteristics can be used as a viable approach to the measurement of the surface temperature, the determination of the presence of water (ice), and the discrimination of minerals. This approach has been used in previous missions including the Thermal Emission Spectrometer (TES) from the Mars Global Surveyor (Christensen et al., 2001a), the Thermal Emission Imaging System (THEMIS) from the Mars Odyssey Mission (Christensen et al., 2004), OMEGA on the Mars Express (Bibring et al., 2005), and the Thermal Emission Spectrometers (TES) on the Mars Exploration Rovers (MER 1 & 2) (Christensen et al., 2003).

A spectrometer measures the intensity of light as a function of wavelength for radiation emitted or reflected from a surface (Wolfe and Zissis, 1978). The wavelengths can be separated by a prism, a diffraction grating, an FTIR, etc.

A bolometer based radiometer measures the energy via the difference between the radiation incident on the detector and a reference level (Wolfe and Zissis, 1978). An example of an instrument is the High Resolution Dynamics Limb Sounder (HRDLS) (Massie et al., 2007). This was designed to provide Earth global temperature and composition data. The incoming radiance is directed by a scan mirror to a primary mirror that is chopped against a cold space reference. The radiance is then directed off the secondary mirror via a folding mirror to spectral band-defining filters. These devices have a good history of use in satellite remote sensing, and

other examples include the Mars Reconnaissance Orbiter (Taylor et al., 2006, Zurek and Smrekar, 2007) and the Lunar Reconnaissance Orbiter (Chin et al., 2007, Paige et al., 2010). Typical components of a filter radiometer are provided in Figure 1-3.

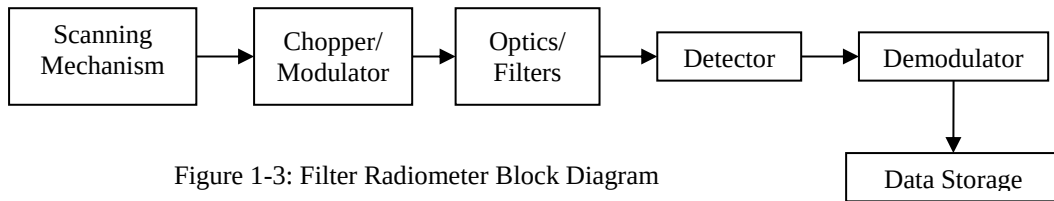


Figure 1-3: Filter Radiometer Block Diagram

Both of these potential instruments have common advantages over other types of instruments: multiple use instrument not reliant on processing physical samples, measurement in the actual environment, providing stratigraphy and context of a borehole for interpretation of extracted samples, and being able to combine with data from other instruments to provide better mineral discrimination. Table 1-7 provides a comparison of the differences for remote sensing.

Table 1-7: Comparative Advantages of the two borehole instrument types.

Instrument	Advantages	Disadvantages
Spectrometer	• Full range measurement of mineral spectra to allow detailed analysis and identification • A survey instrument	• No commercially available components in small borehole diameter (<25 mm). Would require fully custom design and fabrication. • SNR and wavelength transmission losses through a fibre optic cable • Requires full spectral range, collimated light source
Radiometer/Reflectometer	• Extremely low power and compact • Low cost commercially available components • Wide wavelength measurement range • Simple instrument, fewer parts • Can utilize narrow-band IR sources such as LEDs	• Limited data sets to answer full science questions • Not a survey instrument

The spectrometer can measure the full spectra (within the response range of the detector). This is an advantage as a general survey instrument allowing the determination of the mineralogy. Fewer channels in the radiometer/reflectometer design limits the capability to determine the mineralogy. On the other hand, the radiometer has lower size and power resource requirements.

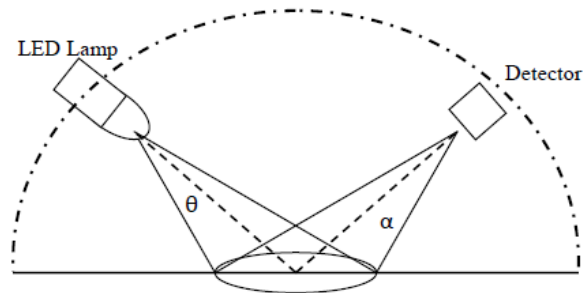
The purpose of this thesis is the determination of the habitability of subsurface icy and soil environments. It is not a general survey instrument. It is being designed to work in

combination with other instruments and datasets (Section 5.8) in order to allow for the detection and classification of water, water ice, hydrated minerals, and temperature. This means that the limited capability to detect the presences of hydrated mineral composition is acceptable and that an IR reflectometer can satisfy the science requirements, as will be discussed in the next section.

1.6 Introduction to radiometry and reflectometry

In the simplest terms, radiometry measures the energy emitted or reflected from a surface in comparison to a reference level (Figure 1-4), with theta (θ) as the angle of incident radiation and alpha

Figure 1-4: Geometry of a Radiometer



(α) as the angle of reflected energy. A detector is required to collect the energy from either reflected or emitted radiation. Emitted energy comes in the form of thermal emission from the surface, while reflected energy requires a source. In natural environments, the reflected energy source is typically the sun; however, in the case of a borehole radiometer, it will require a compact light source to be co-located with the detector.

The spectral range of a radiometer is directly dependent upon the response of the detector. In this application, a filter is required in order to restrict the energy reaching the detector to a frequency band of an absorption feature corresponding to a mineral or water. These filter frequency bands are commonly used for the detection of water, methane and CO₂ in atmospheric measurements, and for surface mineral discrimination. The previous devices are larger than the expected diameter of a borehole (<25 mm), so a

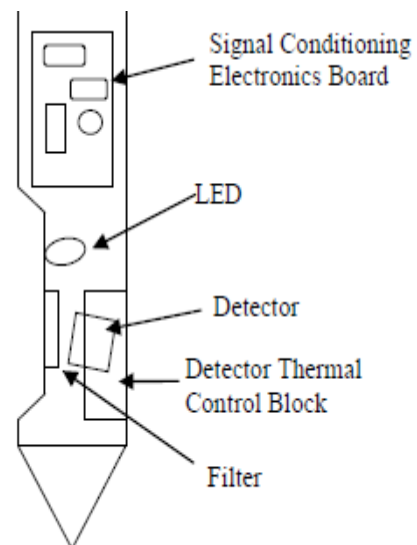


Figure 1-5: Borehole IR Filter Radiometer Concept

major concern in the development of this thesis was to identify miniature components and approaches to build a compact borehole instrument that could meet demanding technical performance specifications (Section 1.3).

A concept for the integrated instrument is presented in Figure 1-5. The integrated borehole instrument will include the detector with thermal control, a filter, LED (for the IR reflectance channels), and amplification circuits. A micro-controller will be located above ground with the power supplies and will be interfaced with a Toshiba Toughbook. This will allow direct control and data collection via the micro-controller.

The development of an IR reflectance filter radiometer involves parallel development in an iterative process. The flow chart in Figure 1-6 provides an overview of the systematic approach to this effort to ensure that the scientific questions and objectives are obtained at the end of the design and analysis process.

This flow has been followed throughout the development of this project. There are several key points that should be mentioned. The Scientific Questions in Table 1-1 set the performance requirements (Table 2-9) for both the mineral and component selection. In all the following steps, the system performance, or the capability for spectral discrimination given Signal to Noise Ratio (SNR) limits, is constantly checked against the

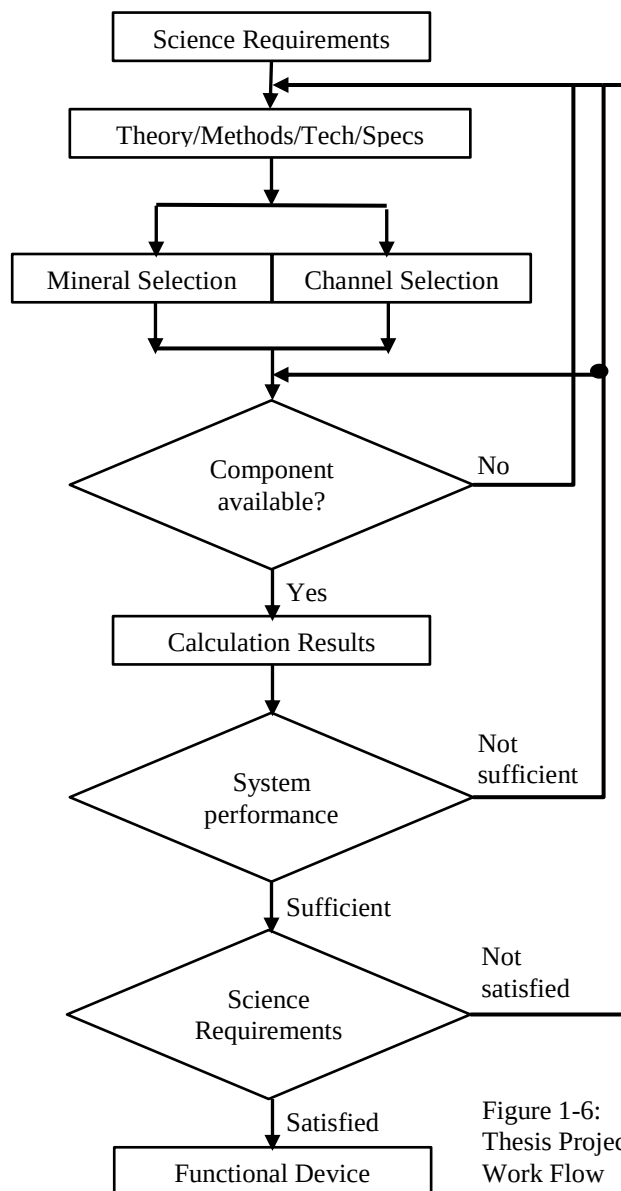


Figure 1-6:
Thesis Project
Work Flow

Scientific Questions. If the questions could not be answered with the results, then a re-evaluation of the channels and mineral and/or spectra was required.

1.7 Methods for the measurement of IR thermal emission and IR reflectance

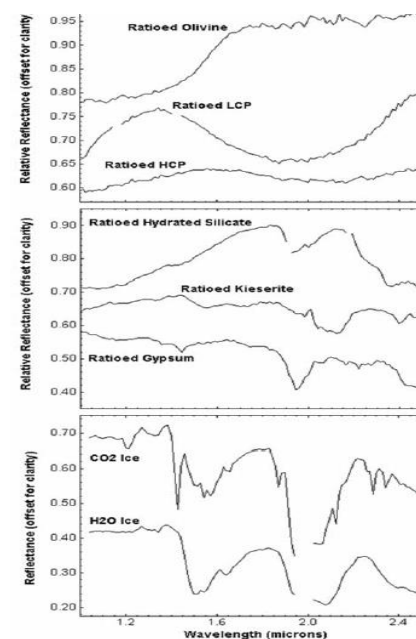
IR reflectance and thermal emission were determined to be the best remote, contactless methods for mineral discrimination, water detection, and temperature measurement (Section 1.5). There is a large body of work surrounding IR reflectance and thermal emission and the reader is referred to works by Houghton & Smith (1966), Wolf & Zissis (1978), and Hapke (2012); however, a brief overview is presented here in order to provide context for the work in this thesis.

Minerals have IR absorption and emission features in their spectra. Spectral features in the visible to near-IR range (~430 to 2500 nm) tend to be due to electronic transmissions between atoms in the crystal lattice (e.g., Fe) while spectra at longer thermal IR wavelengths (e.g., > 5 μm) are dominated by vibrational frequencies associated with stretching of the atomic bonds between the atoms (Farmer, 1974). These absorption features depend upon mineral composition and can be used to discriminate the composition. (Christensen et al., 2000). Additional constituents, such as water content, will absorb known frequency bands and can be used to aid in the discrimination of mineral types such as hydrated minerals or for the direct detection of water (Evdokimova et al., 2009). In thermal emission, regions where the emissivity is close to unity (e.g., = 1) can be used to measure the surface temperature (Sebastian et al., 2010). These represent two complementary methods.

IR reflectance spectra

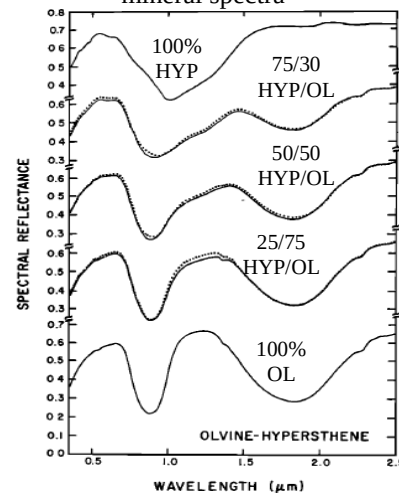
In Visible/Near Infrared (Vis/NIR) reflectance, light reflected off the mineral surface is absorbed in frequencies that are specific to a mineral type and/or the presence of water (e.g., vibrations from OH^- bonds). Figure 1-7 (lower panel) provides an example of mineral

Figure 1-7: Omega instrument sample spectra



spectra including water ice from IR reflection from the OMEGA instrument on Mars Express (Pelkey et al., 2007). Intimate mixture models are required in order to get good compositional information; however, the light reflected off of the surface of an intimate mixture is a nonlinear function of the reflectance of the pure end members (Hapke, 2012, Nash and Conel, 1974). Mineral spectra de-convolution from a non-linear model was

Figure 1-8: Deconvolution of mixed mineral spectra



demonstrated by Johnson et al. (1983) in Figure 1-8. This provides a comparison of measured and calculated spectra of mixtures of olivine (OL) and hypersthene (HYP). The dotted lines represent the calculated values and the solid lines represent the measured values. While the correlation between the calculated mixed models and the measured values are within $\pm 3\%$ spectral reflectance, the divergence demonstrates the unpredictability of multiple reflectance pathways between the particles of the non-homogenously mixed end-members.

Thermal emission spectra

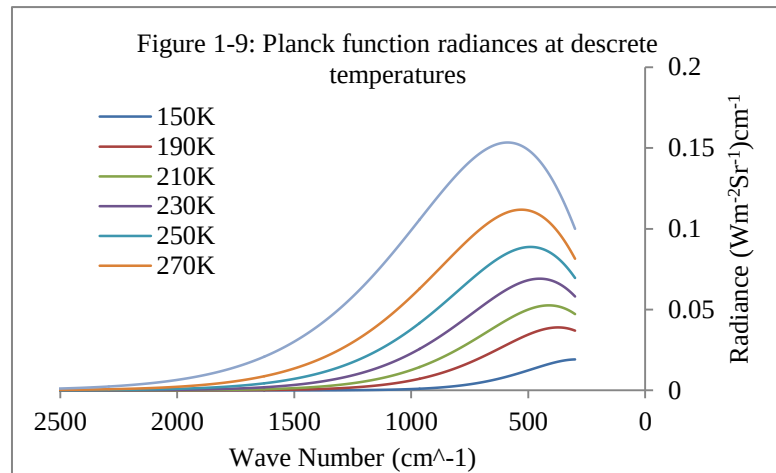
It is known from Planck's law of blackbody radiation that any material above absolute zero will radiate thermal infrared energy. The quantity of energy emitted is dependent upon the temperature and emissivity of the material. The Planck Function (Equation 1-1) can be used to model the energy emitted by wavelength at discrete temperatures:

$$B_{\nu} = \frac{C_1 \nu^3}{\exp\left(\frac{C_2 \nu}{T}\right) - 1} \quad \text{Equation: 1-1}$$

Where: $C_1 = 1.911 \times 10^{-8} \text{ Wm}^{-2}\text{sr}^{-1}(\text{cm}^{-1})^{-1}$; $C_2 = 1.439 \text{ K}(\text{cm}^{-1})^{-1}$; T = temperature of the object, and ν is the wavenumber of the emitted energy.

The result of a typical blackbody series is shown in Figure 1-9 for the expected temperature range on Mars from 150 K to 300 K. This analysis assumes that the emissivity of the surface is at unity, though the actual surface emissivity will vary. Both IR thermal emission and

IR Reflectance methods were utilized in this project in order to answer the questions posed in Table 1-1.



1.8 Overview of numerical performance models

An important component to this project was to generate infrared (IR) emission, IR reflectance, and integrated numerical models to demonstrate that the measured results of a field device match the predicted calculated results. Three different model types were generated and each had specific data requirements. These are presented in detail in Chapter 4; however, they are briefly described here in order to provide a basic understanding of what information is necessary for selection and testing of analogues (Chapter 2) and technology (Chapter 3). The detailed methods and algorithms were developed in Chapter 4. Chapter 5 expanded these to the integrated borehole instrument. These were compared to an integrated bench-top system in Chapter 6.

Thermal Emission

The thermal instrument model is based on thermal radiation emitted from the surface material and includes temperature variations in the instrument. This energy passes through the filter and window and is converted into voltage by the detector. The voltage is then converted into radiance that can be correlated to the temperature of the surface. Section 4.2 will address the general thermal model. Chapter 5 will consider the component performance and will allow the calculation of a noise/error that can be used to determine the performance and limitation of the thermal channels in the integrated instrument. Data required includes the detector performance specifications (defined in Section 3.3), filter/window transmission characteristics, and material emissivity (including a calibration target).

Reflectance

Basic: Pure minerals

Analysis of the spectra for a pure mineral provides a straightforward means of demonstrating the specific features related to hydrated minerals and water ice at 1.4 and 1.93 μm . This is the first step in validating the integrated system models and calculations. This required measurement of pure mineral spectra from 1-3 μm . This is described in detail in Section 4.3.

Linear mixing

Linear mixing models have been used as a means of de-convolving measured mineral spectra in the thermal IR (Ramsey and Christensen, 1998) and in the Near-IR (Combe et al., 2008). This is a simplified approach in which mineral spectra are combined by weighted average according to the mixing ratio of two or more pure minerals (Singer and McCord, 1979).

In the thermal IR range ($> 5 \mu\text{m}$), spectrally mixing is potentially more straightforward because of independent oscillations from the mixed minerals, limited photon reflection pathways (reducing multi-surface reflections), and Reststrahlen bands emitting from the top layer only (with the additional assumption of particles sizes $> 100 \mu\text{m}$) (Ramsey and Christensen, 1998). Previous missions utilizing this approach include the Mars Global Surveyor Thermal Emission Spectrometer (TES) (Christensen et al., 2003) and Mars Odyssey Thermal Emission Imaging System (THEMIS) (Christensen et al., 2004)

An example of the use of linear-mixing models in the near-IR reflectance range (1 to 2.5 μm), this approach is for data from the OMEGA (Observatoire pour la Mineralogia, l'Eau, Les Glaces et l'Activite) instrument (Combe et al., 2008). A key assumption for linear mixing in the near-IR, and limitation, is that the end-member materials must be in physically discrete patches because intimate mixtures cause non-linear multiply scattered incident light at the surface (Combe et al., 2008, Hapke, 1981, Hapke, 2012). While the results of linear mixing are expected to be insufficient for the modelling necessary for this thesis (Keshava and Mustard, 2002), as a first pass of the analysis, linear mixing models were generated in the near IR range in order to compare a linear weighted combination of mineral spectra with spectra of physically mixed samples. This

required measurement of pure and mixed mineral spectra from 1-3 μm . This is described in detail in Section 4.4.

Hapke (non-linear mixing)

Because the spectral characteristics of individual minerals do not combine linearly in the near-IR, a more complex model is necessary to confirm the capability to discriminate mineral mixtures. The models of Hapke were developed for the reflectance spectra of particulate surfaces of intimately mixed minerals (Hapke, 1981, Hapke, 1984, Hapke, 1986, Hapke et al., 1993). This has evolved over the last decade or so to be the most accepted method for modelling mixed mineral spectra. An alternative method developed by Shkuratov avoids some of the key assumptions and limitations of the Hapke model; most directly by incorporating realistic grain forward scattering at all orders of scattering (as opposed to only to the first order in the Hapke model) (Poulet et al., 2002, Shkuratov et al., 2012). For this thesis, a Hapke model will be used to generate synthetic spectra for a limited set of mineral and water ice examples to demonstrate the limits of de-convolving intimately mixed minerals with the proposed instrument. The particle size distribution, mineral density, and indices of refraction (real and imaginary components) are required for each of the materials to generate the Hapke model. This is described in detail in Section 4.5.

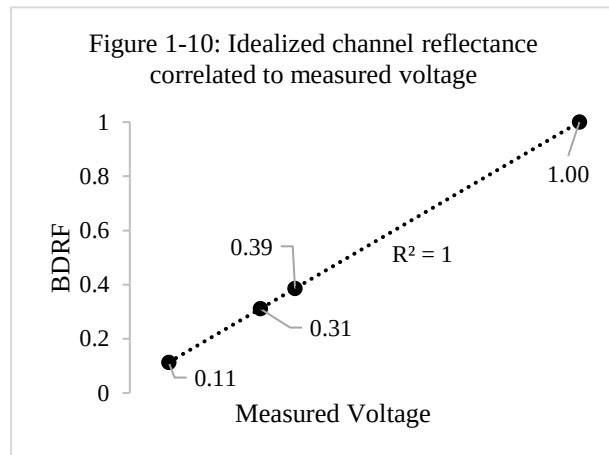
Integrated system models

Integrated system models will be presented in Chapter 5. Component performance characteristics were evaluated with the spectral characteristics of the materials in order to produce an integrated system model. Both the thermal IR measurements channels and the IR reflectance channels were modelled independently. The theoretical performance calculations of an IR reflectance filter radiometer were based on the measured performance of the selected components and the measured reflectance spectra (R) of the selected minerals. The emission spectra were generated from measurement of the reflectance spectra as $(1-R)$ in biconical reflectance. Required data included measured data on the components, mineral spectra, and experimental set-up and characteristics. This is described in detail in Sections 5.2 (thermal channels) and 5.4 (reflectance channels).

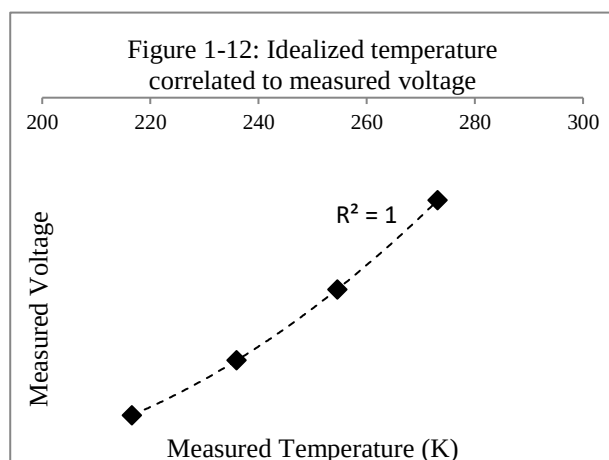
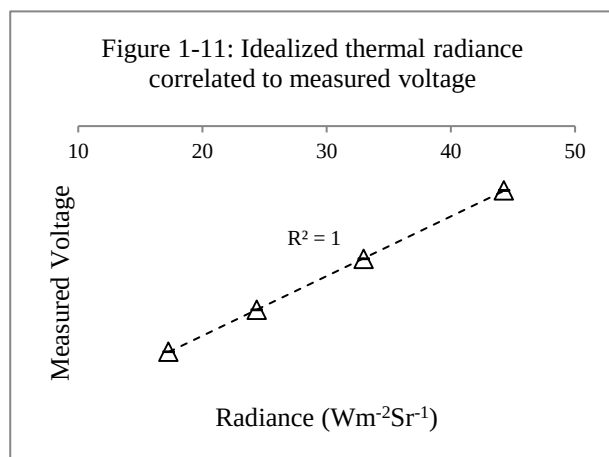
1.9 Overview of measurement, calibration, calculations, and expected results

The primary output of this instrument is a voltage based on the emitted or reflected energy reaching the detector. Models were developed and calibration techniques established in order to convert this voltage into a relative reflectance or temperature.

Idealized calibration curves for reflectance and thermal IR emission are shown in Figures 1-10 and 1-11, respectively. In Figure 1-12, the Bidirectional Reflectance Distribution Function (BDRF), or the amount of reflected energy reaching the detector, can be correlated to the measured voltage.



Similarly, in Figure 1-11, the emitted energy in the form of radiance can be correlated to the measured voltage. The relationship of measured voltage to radiance is the important relationship to demonstrate that the calibration of the thermal IR system is valid; however, the conversion of voltage to temperature can be determined directly by plotting the voltage generated from the measurement of a surface with a known emissivity and temperature (Figure 1-12). Because the fit of this data is a polynomial of the temperature, the easiest way to convert voltage to temperature is to create a look-up table for temperatures in the



expected performance range with a reasonable resolution (0.1 K for the purposes of this thesis). The generated voltage is then used to look-up the expected surface temperature.

When properly designed and calibrated, voltage plotted against radiance is a linear relationships (Figure 1-11). Calibration via models and measurements of calibration standards with known reflectance and emission characteristics, as well as the temperatures of these surfaces, was a critical part to the design and assessment of instrumentation performance. Creating an experimental design with known characteristics was also an important part of the validation of the methods, technology, and instrumentation.

Experiments and models were developed iteratively. Primary methods and equations remained constant through each iteration, with the iteration designed to improve the instrument performance, the experimental design to more closely match a borehole configuration, or the models to match updates to the component, instrument, or experimental design. There were a number of challenges to correlating the predicted to measured values: 1) Everything that attenuated the energy reaching the detector had to be accounted for (such as the geometry, windows, and filters). 2) Everything that added energy reaching the detector (such as components within the Field Of View (FOV) of the detector and energy beyond the FOV reflected off of the sample surface into the detector). 3) Thermal variations of the detector and LEDs. 4) Electrical noise. 5) Component performance limitations. These were all managed systematically and iteratively in the integrated models (Chapter 5) and instrument testing (Chapter 6).

1.10 Mars Reference Mission

As an additional guide to the development of this project, it is useful to consider it in the context of what a Mars mission might look like. Table 1-8 presents a proposed Mars Reference Mission in which this instrument could be used. This is compared to what configurations will be tested in laboratory and natural environments to demonstrate the capability for this technology solution to meet the science requirements.

Table 1-8: Mars on Earth reference mission compared to thesis testing

Mars Reference Mission	Laboratory Testing
1. Rover 2. Retractable Sensor Pod 3. Seated in Cradle when not deployed a. Calibration targets in Cradle 4. Calibration in Cradle pre and post deployment 5. Pre-measurement of surface materials a. Bore-hole radiometer through viewing port in cradle b. Other Assets: i. PanCam equivalent ii. Spectrometer iii. Satellite 6. Pre-measurement of bore-hole cuttings a. Bore-hole radiometer deployed with a surface cone attachment b. Other Assets: i. PanCam equivalent ii. Spectrometer	1. Phase A: Flat Surface a. Sensors/LEDs mounted above a flat surface: i. Bread board design ii. Integrated bore-hole design b. Calibration pre and post measurement of a single material. c. Results compared to spectrometer readings of the same material d. Temperature: With vacuum and cycling of material temperature e. Mineral IR Reflectance: No vacuum and no cycling of material temperature 2. Phase B: Bore-hole simulator a. Sensor pod inserted into simulated bore-hole i. Packed minerals as flat surface ii. Calibration pre and post measurement iii. Results compared to spectrometer readings of the same material whenever possible iv. Temperature: with vacuum and cycling of material temperature b. Mineral IR Reflectance: No vacuum and no cycling of material temperature

1.11 Thesis progression and chapter outline

This thesis started with identifying and characterizing appropriate analogue environments and materials. These were used to determine the performance specifications of individual components and for an integrated system. Individual components were tested to meet the performance requirements and then tested as a bench-top system with analogue samples. Results were used to update requirements and design, build, and test a prototype device in laboratory simulated analogue environments. At every step of the process, results were compared to the original science requirements in order to ensure that the final design would function as expected.

The following chapters will present the full thesis development:

- Chapter 2: *Methods of Measurement, Analogues, sample collection, & Characterization, and Channel Selection to meet science requirements.*
- Chapter 3: *Component selection, testing, and engineering models*
- Chapter 4: *General theoretical models*
- Chapter 5: *Integrated theoretical models*
- Chapter 6: *Bench-top prototype models, testing, and comparison to integrated theoretical models.*
- Chapter 7: *Future Work*

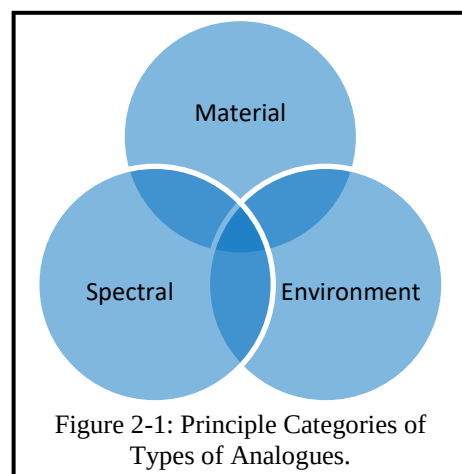
Chapter 2: Analogues, sample collection, characterization, and channel selection to meet science requirements

2.1 Introduction

Central to the success of this thesis was the use of analogue materials and environments for simulating Mars and materials found on its surface. These were used for the development of methods, models, performance requirements, and testing of sensor systems designed as part of this project. The selection of these was guided by the science requirements (Table 1-4), the environmental requirements (Table 1-2), and the types of aqueous altered materials found on Mars (Table 1-3). Section 1.8 defined what models were built and their data requirements. In this chapter, minerals were selected and characterized. The collected data were used to select channels for the instrument and to determine performance requirements for the main components (detector, filter, LED) as well as the integrated system.

2.2 What are Analogues, how are they qualified, and how can they be used?

The use of analogues, simulants and/or natural, is one of the most powerful tools available because access to actual materials is limited (as in the case with lunar materials) or near non-existent (as in the case of Martian materials) (Seiferlin et al., 2008). Their use has become commonplace throughout the community and will be central to the development and testing of hardware in this thesis. One way to organize the division of the variety of analogue types is by material properties, spectral properties, and environment (Figure 2-1). Material properties comprise the physical characteristics of the material (e.g., density, particle size, mechanical strength, chemical composition, etc.). Spectral comprise light reflectance and emission properties of the material. Environment analogues simulate or approximate the expected



conditions in the actual environment. Environmental properties are central to the classification of the habitability of a specific environment.

These three categories are used to group the properties that define and qualify a material and environment (simulated or natural) as an analogue, and under what conditions they may be used. There are many characteristics (Table 2-1) and any one material or environment could simulate one or more of these at once.

Table 2-1: Detailed Listing of Measurable Characteristics of Analogues

<u>Material</u>		
<i>Chemical</i>	<i>Physical: General</i>	<i>Physical: Thermophysical</i>
• Dielectric Constant • Redox Potential • pH • Electric Conductivity • Volatiles • Mineralogy	• Particle Size • Particle Shape • Relative Density • Total Density • Porosity • Water Content	• Albedo • Thermal Inertia
<i>Mechanical</i>	<i>Physical: Geological</i>	<i>Magnetic</i>
• Cohesive Force • Internal Angle of Friction	• Morphology • Geologic Processes • Depth of Layer	• Magnetic Susceptibility • Magnetic Saturation
		<i>Organic</i>
		• Total Organic Carbon • Molecular Abundance • Microorganism Content
<u>Spectral</u>		<u>Environment</u>
• Diffuse reflectance • Bi-Directional reflectance • IR (near, mid, and far) (700 nm – 100 µm) • Visible reflectance (390-700 nm)		• Temperature • Atmospheric Composition • Atmospheric Pressure • Ultra-Violet irradiation

*Note: Table compiled from Valdivia (2008), Marlow et al. (2008), and Sabille & Schlagheck (2005).

Environments

Analogue environments include both simulated and natural settings. The requirements for these were described in section 1.2 and Table 1-2.

Simulated

Simulated environments (Figure 2-2) will be used in this project to test methods and hardware at Mars temperatures in order to ensure that results match what the instruments would see on Mars. These environments will be combined with Mars analogue materials for some of the tests.

Natural

Recent years have acknowledged the limitations in the use of analogue materials in laboratory settings as their removal from their natural environment quite often changes the very nature that resembles another planetary body such as microstructure, humidity, natural temperature, pore space, ambient pressure, and other key parameters (Seiferlin et al., 2008). Mars is dry and barren and simulated environments cannot test hypotheses, methods, and technology in the same way as can be tested in natural environment on Earth that closely matches an aspect of Mars; however, qualification of natural analogues must be clearly defined for a specific environment and purpose.



Figure 2-2: Chamber at AOPP that was used to Simulate Mars Environmental Conditions.

There are few natural analogue environments to cold, dry Mars (Figure 2-3). As the environment moves from wetter to drier and from warmer to colder, frozen, pure water will convert directly to vapour as indicated by the dashed line in Figure 2-3. Mars, at its highest expected obliquity of 45° (implying the complete evaporation of the polar CO_2 caps during this period), just crosses under the line as atmospheric pressure is increased combined with warmer surface temperatures (Carr, 1996, Laskar et al., 2002). At low obliquity of 25° , only special conditions or increased water salinity will allow the formation of liquid water on the surface because the atmospheric pressure and temperatures will be too low to allow for liquid pure water.

There are many other locations throughout the globe that provide analogue materials, and it is important to test *in situ* whenever possible, even when the

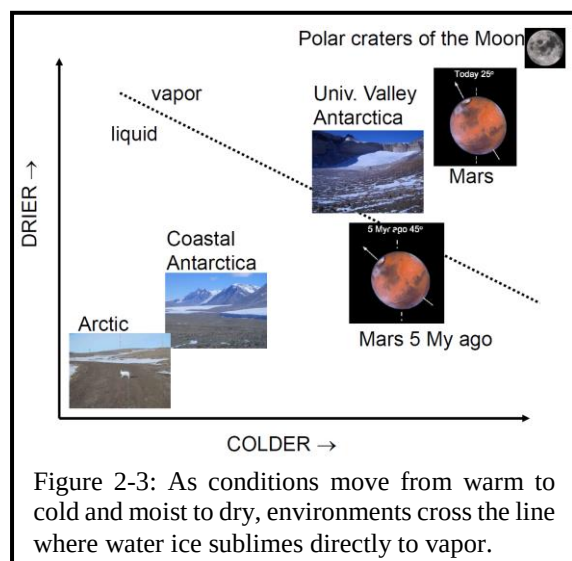


Figure 2-3: As conditions move from warm to cold and moist to dry, environments cross the line where water ice sublimates directly to vapor.

environmental conditions do not match Mars. Ideally, instrumentation should be tested in appropriate natural analogue environments as a step towards development for future flight opportunities (Future work, Chapter 7).

Analog Material Selection

Material analogues will be used to test and validate the design of sensors to measure the spectral signatures of similar materials to those found on Mars. These will also be used to build the IR reflectance, linear mixing, Hapke, and integrated models. A preliminary discussion of these was presented in section 1.2 and Table 1-3; however, there is a significant body of work in the literature detailing the detection and identification of a variety of materials on the Martian surface that is beyond the scope of this thesis. The reader is referred to several papers for additional information (Ehlmann et al., 2010, 2009, Mustard et al., 2008, Pio Rossi and van Gasselt, 2010); however, Table 2-2 provides a detailed summary of these materials, where they have been found on the surface of Mars, their terrestrial analogue equivalent (with location), and references. Figures 2-4 and 2-5 mark where some of the locations where these are found on Earth and Mars, respectively.

These minerals include those that contain C, H, O, N, P, & S that are necessary for building cellular material; those that can be utilized as a chemical energy source; those that were formed through an aqueous process (indicating liquid water on the surface of Mars); and those that provide a current niche habitat (such as salts).

The subset of materials selected for this project are marked in Figures 2-4 and 2-5 with stars, coloured according to the key in Table 2-2. Of the 13 samples selected, the montmorillonite, halite, and gypsum samples were purchased from Wards Natural Sciences Company. GPS coordinates and source are provided when they were available. The quartz samples were purchased from Fisher Scientific and the Acros Chemical Company, and JSC Mars-1 was provided by NASA. All other samples were collected during field expeditions to the Mojave Desert, Panoche Hills, the Eastern Atlas Mountains, Morocco, and the Rio Tinto, Spain.

Figures 2-4 & 2-5: Comparison of Similar Materials Found on Both Earth and Mars

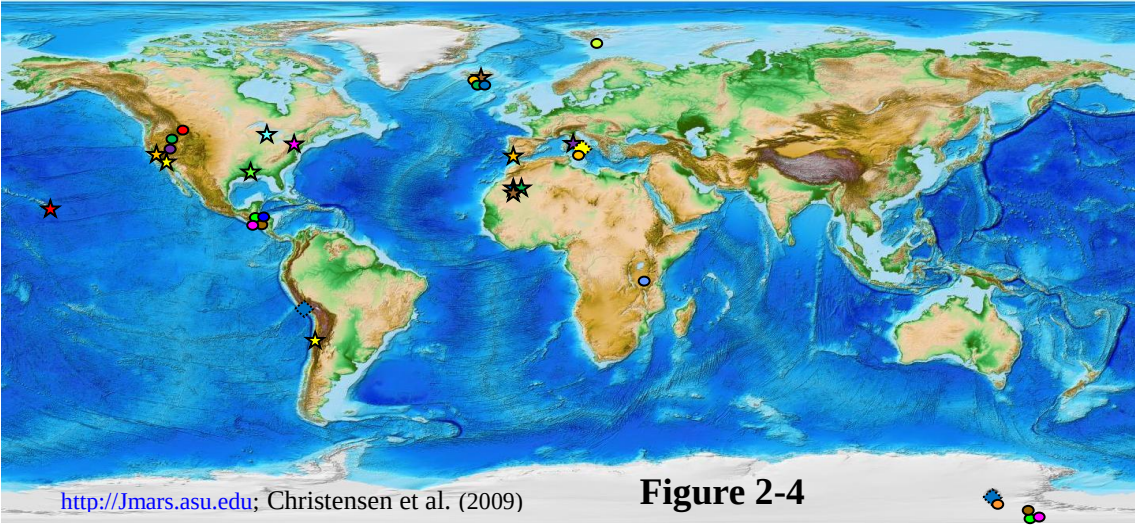
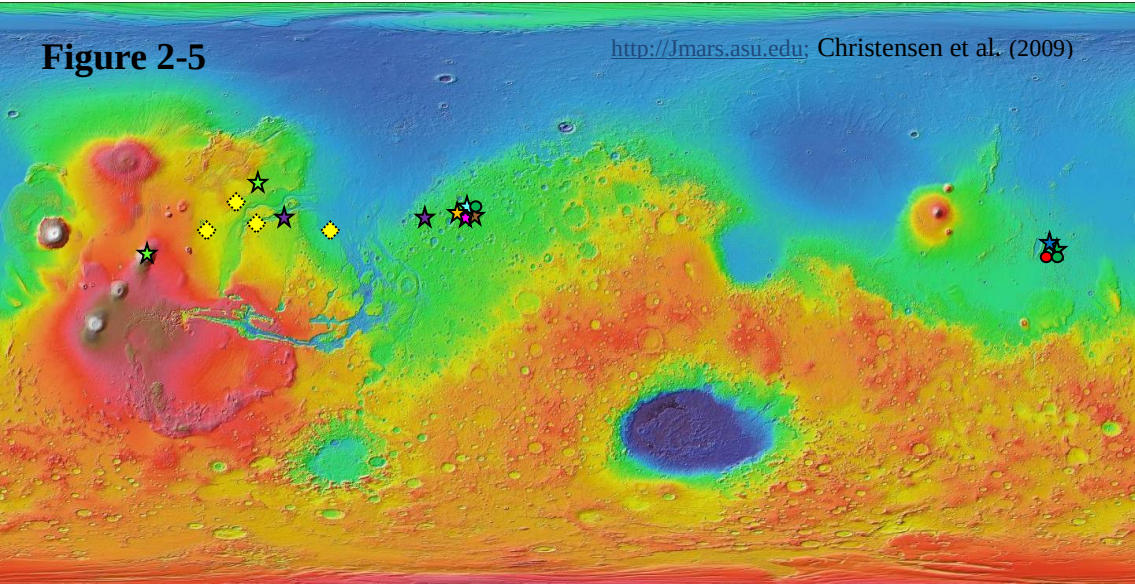


Table 2-2: Location of Similar Materials Found on Both Earth and Mars

Sample		Location: Earth	Location: Mars	References
Ca-carbonate (2)	★	Morocco	Gusev Crater	Boynton et al. (2009)
Basalt (2)	★	Morocco, Iceland	Meridiani Planum	Rieder (2004)
Gypsum	★	Pomaia, Italy	Juventae Chasma, Iani Chaos	Gendrin (2005)
Limestone	★	Morocco	-	Earth Only
Halite	★	Hampton Corners, NY, USA	Meridiani Planum	Bridges & Grady (1999) Rieder (2004)
Jarosite (2)	★	Panoche (USA), Rio Tinto (Spain)	Meridiani Planum	Golden et al. (2008)
Quartz (2)	★	Purchased from Fisher & Acros	Generally Abundant	Bandfield (2002)
JSC Mars-1	★	Pu'u Cinder Cone, Hawaii, USA	General Spectral	Morris et al. (1993)
Montmorillonite	★	Panther Creek, MS, USA	Syria & Lunae Planum	Bishop(1993)
Hematite	★	Republic, Michigan, USA	Meridiani Planum	Christensen et al. (2001)
Desert Sand (9)	★	Mojave, California, USA Atacama (Chile)	Generally Abundant	Allen et al. (1998) Fletcher et al. (Submitted)
Future Samples (3)	◆	Desert Sands: Peru, Antarctica Sulphates: Italy (Naples Solfatara)	Generally Abundant Ius, Hebes, Capri, Candor	Allen et al. (1998) Gendrin (2005)
Other Analogues	○	Various	Various	Appendix B

Note: Stars = Samples Already Collected; Diamonds = To Be collected; Circles = others as necessary.



2.3 Analog Material Collection and Characterization

The material analogues for this project were selected for use as spectral analogues. Preparation and characterization of these samples was performed to ensure a proper spectral signature for use in the

Table 2-3: Characterization Tests for Material Analogues

	Property	Method	Justification
Physical	Particle Size	Dry sieve separation	Particle size changes the spectral features. Common size fraction for comparison to other similar samples.
Spectral	Diffuse Reflectance	Mid/Near IR	Principle measurement for characterization of material analogues. Used for determination of diagnostic bands. Comparison to data from other sources (ASU, RELAB, etc.).
	Indices of Refraction	Literature	Necessary for Hapke model

development and testing

of the hardware and models necessary for this thesis. Information necessary were the physical size and spectral characteristics. Table 2-3 identifies the property that is needed to be understood, the methods for measurement, and the justification for that data. Details for each of the samples collected as part of this project are provided in Table 2-4.

All samples except the basalt were considered pure and standard chemistry indices of reflection obtained from the literature are used (Table 2-5). The basalt sample had additional SEM and EMP testing to determine the chemistry. All samples had spectral measurements made at RELAB (Brown University). Methods and results are described in the following sections.

Preparation of Powder Samples

Several of the samples obtained for this project were in the form of rocks or large grain form. These included the basalt, gypsum, limestone, halite, and both the jarosite and Ca-carbonate samples. For the initial survey of mineral band positions, these needed to be prepared for spectral analysis by first grinding them into discrete size fractions as described below.

Quantities of each mineral as collected were saved so that sensors will be able to be tested against the minerals in their natural forms. Each sample was first cut into small pieces with a rock splitter (Figure 2-6A) and then passed through a rock crusher (Figure 2-6B) multiple times,

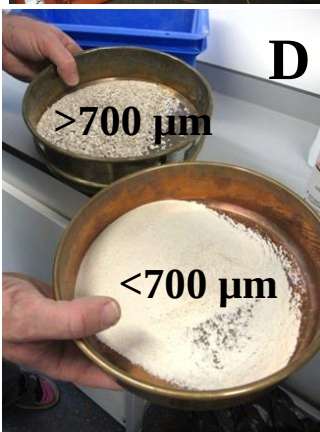
closing the diameter of the throat with each successive pass until reaching the smallest throat size (Figure 2-6C). All equipment and machinery were thoroughly cleaned with isopropanol in-between each sample in order to reduce cross sample contamination.

Table 2-4: Details of collected material analogues

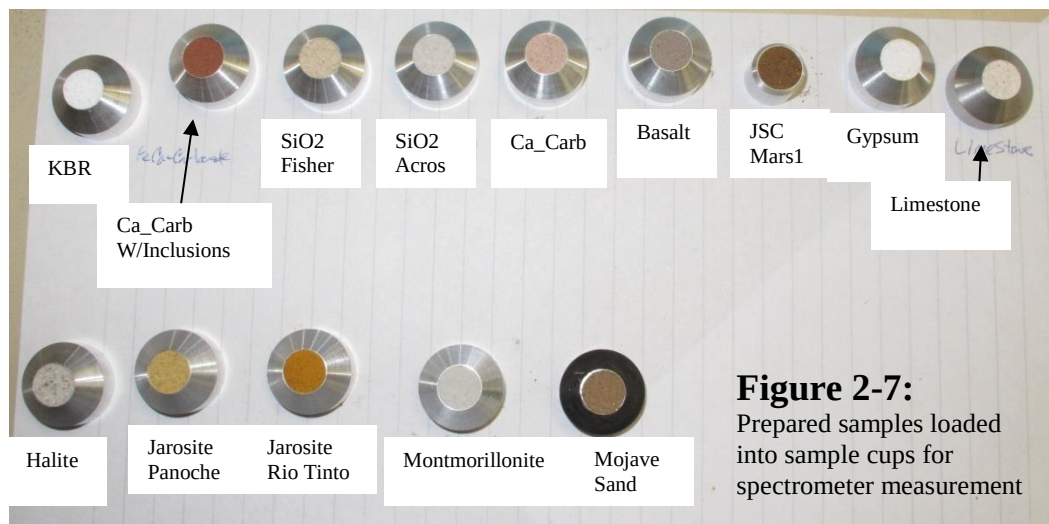
Sample	Location	GPS Coordinates	Description	Mars References
Ca-carbonate	Morocco	31° 22.791' N 04° 01.894' W	Kess Kess Mud Mound	Morris et al. (2010)
Ca-carbonate w/Fe inclusions	Morocco	31° 22.724' N 04° 01.905' W	Kess Kess w/inclusions	Morris et al. (2010)
Basalt	Morocco	31° 25.979' N 05° 38.981' W	Pure flow	Rieder (2004)
Gypsum	Pomaia, Italy	43° 25' 23.75" N 10° 33' 19.09" E	Wards P/N: 46E 3783	Gendrin (2005)
Limestone	Morocco	30° 59.365' N 06° 41.972' W		Morris et al. (2010)
Halite	Hampton Corners, NY	42° 44' 49.25" N 77° 58' 13.73" W	Wards P/N: 46E 3828	Bridges & Grady (1999) Rieder (2004)
Jarosite	Panoche Hills, CA	36° 37'08.18 N 120° 39' 15.98" W	Pure vein, sub-surface	Golden et al. (2008)
Jarosite	Rio Tinto, Spain	37° 37' 39.90 N 6° 32' 10.78" W	River bed sample	Golden et al. (2008)
Quartz	N/A	N/A	Fisher P/N: S25-3	Bandfield (2002)
Quartz	N/A	N/A	Acros P/N: S24/25	Bandfield (2002)
JSC Mars-1	Pu'u Cinder Cone, Hawaii	19° 43' 14.13" N 155° 28' 19.54" W	Orbitec	Allen et al 1998
Montmorillonite	Fowlkes Mine, Panther Creek	33° 45' 09.29' N 88° 31' 43.49" W	Wards P/N: 46E 0435	Bishop(1993)
Mojave Sand	Little Red Hill, CA	35° 22'15.22" N 116° 09' 48.06" W	Arid environment	Allen et al. (1998) Fletcher et al., 2011 a&b



Figure 2-6: A) Rock Splitter, B) Split pieces fed through the grinder, C) Subsequent passes at smaller throat diameters, D) Final >700 μ m and <700 μ m.



Samples were first separated into $>700\ \mu\text{m}$ and $<700\ \mu\text{m}$ size fractions (Figure 2-6D). These were later dry sieve separated into additional size fractions. These were $<90\ \mu\text{m}$, 990-500 μm , 500-710 μm , 710-1000 μm , 1000-1400 μm , and $>1400\ \mu\text{m}$.



The size fraction used for all testing of hardware was 710-1000 μm . This was a common size fraction used by a number of other researchers for Mars-like analogues (RELAB database). The resulting samples are shown in Figure 2-7.

IR diffuse reflectance characterization

Mid and Near IR Diffuse Reflectance were measured for each of the samples at RELAB (Brown University). The RELAB facility at Brown University provides a mechanism for researchers to obtain high quality laboratory spectra of geologic materials for use in compositional and/or geologic applications (Pieters and Hiroi, 2004). Samples were sent to RELAB for measurement for mid and near IR diffuse measurement according to their standard internal procedures as follows: The principal instrument was a Nicolet 870 Nexus FTIR spectrometer for near- to far-infrared measurements. The system included a Pike diffuse reflectance accessory. All samples were measured from 1-50 μm . All ratios were adjusted using the National Bureau of Standards (NBS) Halon calibration table.

Characterization of basalt sample

The basalt sample collected from the Tinerhir site was characterized at the University of Oxford Materials Science Laboratories at the Begbroke Science Park. Bulk chemistry and mineral

distribution in the unknown mixed sample were determined with scanning electron microscopy (SEM), SEM with energy dispersive X-ray (EDX) analysis, and electron micro-probe (EMP) analyses Appendix F).

The rock was predominantly a combination of pyroxenes (diopside & augite from XRD) and nepheline, with the epidote mineral clinozoisite (from XRD). In addition, the SEM analysis showed the presence of apatite at level to bring the mean phosphorus oxide content to above 2%. In addition, titanium containing minerals were relatively common, including various iron-titanium oxides and more occasional perovskite $(\text{Ca,Na,Fe,Ce})(\text{Ti, Nb})\text{O}_3$. This information was used to select optical constants necessary for the Hapke model as part of Chapter 4.

Optical constants for Hapke models

Hapke models will be generated in Chapter 4 for non-linear mixing of a sub-set of the minerals collected for laboratory testing. Table 2-5 includes the optical constants (real and imaginary components), the material density, and the source of the data. For the models, optical constants are wavelength dependent and vary from 1-2.5 μm .

Table 2-5: Material Optical Constant and Density Data

Sample	Indices of Refraction in 1.25 to 2.1 μm wavelength range		Material Density g/cm ³	Reference
	<i>n</i>	<i>k</i>		
Basalt	1.51	$(1.8 - 2.8) \times 10^{-3}$	3.36	Modelled as a Palagonite Tuff (Clancy et al., 1995)
Gypsum	1.500 – 1.531	$10^{-3} - 10^{-5}$	2.31	(Roush et al., 2007)
Mars JSC-1	1.5	10^{-5}	2.59	Modelled as a Palagonite Tuff (Clancy et al., 1995)
Pyroxene	1.72	10^{-4}	3.25	Data provided by Roush, T.
Water Ice	1.3-1.7	$10^{-3} - 10^{-5}$	1.56	(Warren, 1984)

2.4 Additional centralized mineral spectral databases

Early work of this project included the collection and characterization of a limited set of minerals that could be used for follow-on laboratory testing. A more extensive set was needed; however, for testing the theoretical calculations to determine if the scientific questions (Table 1-1) can be answered with the proposed system. Collection, processing, and characterization of

physical samples is time consuming, so the spectra for the minerals listed in Table 2-4 were supplemented with mineral spectra from other publically available databases. These databases include those by Arizona State University (Christensen et al., 2000), Brown University (RELAB) (Pieters and Hiroi, 2004), the ASTER spectral library (Baldrige et al., 2009), and the US Geological Services Spectral database (Clark et al., 2007). For the purposes of this thesis, the USGS spectral database served as the primary source for additional mineral spectra.

USGS Spectral Database cross-referenced to minerals on Mars

The USGS Spectral Mineral Database has a well developed and characterized set of 216 minerals and substances. These materials were typically measured at the USGS facility, using uniform methods for sample handling and preparation, spectral measurement, and mineral identification by SEM, TEM, microprobe, or other complementary analytical method. It is for the level of confidence in the accuracy of the datasets that this database was chosen as the primary source of supplemental spectra.

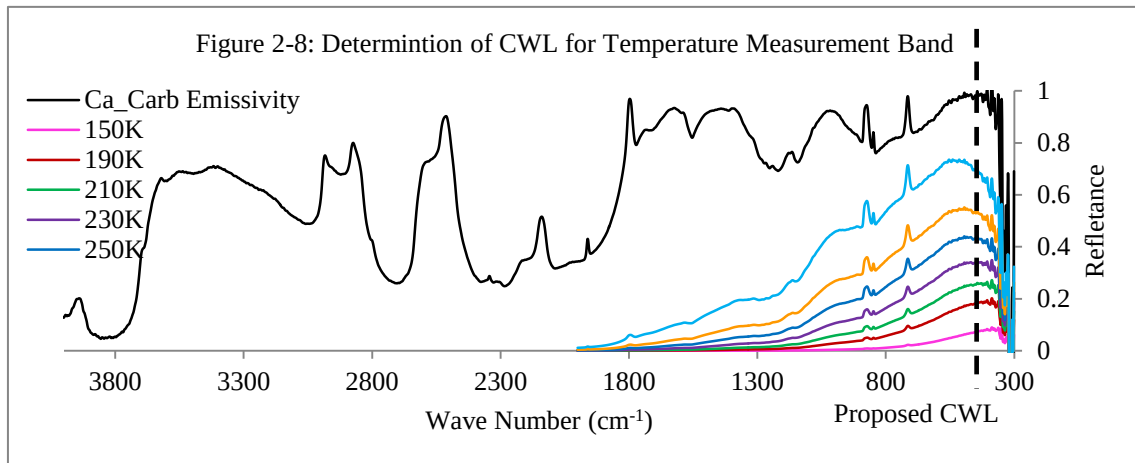
Each of these were cross-referenced to the literature. Ehlmann, et. al., (2013) and Ehlmann and Mustard (2012) , are good sources for an analysis of hydrated minerals found on the surface of Mars, but the full cross-referencing is provided in Appendix D. These were then reviewed and sorted by the following criteria: 1) if it has been found on Mars, 2) Hydrated or not, and 3) mineral type. The 31 minerals resulting from this down selection were used for the forward radiative transfer model calculations as detailed in Chapter 4.

2.5 Selection of IR thermal bands

The determination of surface temperature can be made from the measurement of IR thermal emission, so the selection of thermal emission bands is the first step in developing the IR thermal radiometer portion of this thesis. These bands were used to select corresponding detectors and filters.

The emissivity of the material changes the brightness temperature seen by the detector, so in order to minimize temperature errors, a careful consideration of the expected minerals to be

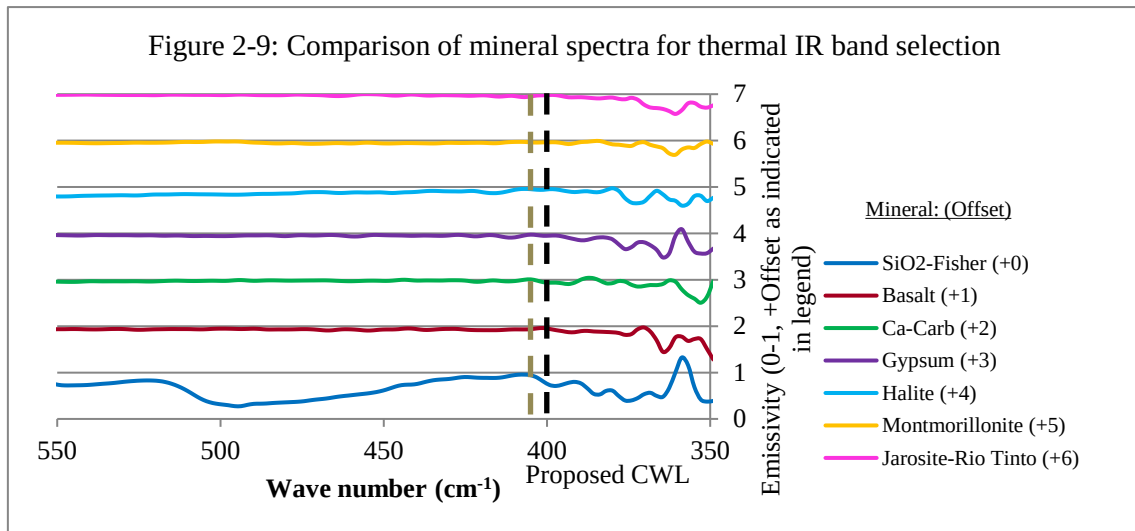
encountered must be made (see previous section). A model was developed by multiplying the thermal emissivity spectra by the Planck function (Equation 1-1) for temperatures from 150-300K at 20K intervals (per proposed environmental range in Table 1-4 and performance requirements, Table 3-8)). Figure 2-8 provides an example spectrum for the calcium carbonate sample collected from Morocco. Synthetic thermal emission spectra were generated for this temperature range.



Note: 1) A factor of five was applied to synthetic emission spectra to allow a visual comparison to the calcium carbonate spectrum.

A final consideration is that the majority of minerals in the sub-surface (at less than five metres depth) will likely already have been characterized from surface measurements (discussed in detail in Section 5.8). This prior knowledge of surface materials can be used to aid the selection of the channel frequency position. The approach for this thesis used a single sensor fitted with a filter (Figures 1-5 and 6-4). The filter was selected to allow energy to pass from a frequency range associated with a high material emissivity taken from known minerals on the surface of Mars. The frequency range of this band-pass was selected to optimize the collected emitted energy. The Centre Wavelength (CWL) for this occurs at about 400 cm^{-1} for the lowest temperature of 190 K (Figure 2-8).

Expanding this evaluation for a larger set of minerals, the spectra for seven minerals are compared for the spectral range from 350 to 550 cm^{-1} in Figure 2-9 (six have been offset for clarity). As can be seen, the original estimate of around 400 cm^{-1} (black dashed line) provides a good CWL; however, this location is slightly depressed (lower than emissivity of 1) for most samples and especially for quartz (SiO_2), even though finding pure quartz on Mars is unlikely as



it would most likely be mixed in with other minerals. Moving the CWL to 408/410 (brown dashed line) would reduce the errors associated with emissivity variations. The other important decision for reduction of emissivity variation errors is to make the width of the band around the CWL as narrow as possible, while still allowing enough energy to pass to meet the responsivity limits of the detector. Balancing these considerations, along with finding available hardware, becomes an important part of the engineering design and testing phase of this thesis (Chapters 3 and 6).

2.6 Selection of IR reflectance bands

Selection of IR reflectance bands was the first step in developing the IR reflectometer portion of this thesis. This was considered for the detection of water ice and hydrated minerals separately. Absorption peaks are first considered, but in order to detect an absorption feature, the absorption band must be combined with nearby portions of the continuum on either side that do not absorb (Bandfield et al., 2003, Glotch et al., 2010, Parente et al., 2011). For this thesis, these continuum bands are called “anchor” bands (Parente et al., 2011).

Selection of water absorption bands

The fundamental assumption in the project is that there is/was water on the surface of Mars which would be available for biosynthesis or which is indicative of long periods of liquid water on the surface. This involves the identification of either water ice or aqueous altered materials (Table 1-3). Aqueous altered materials are hydrated minerals that are formed under

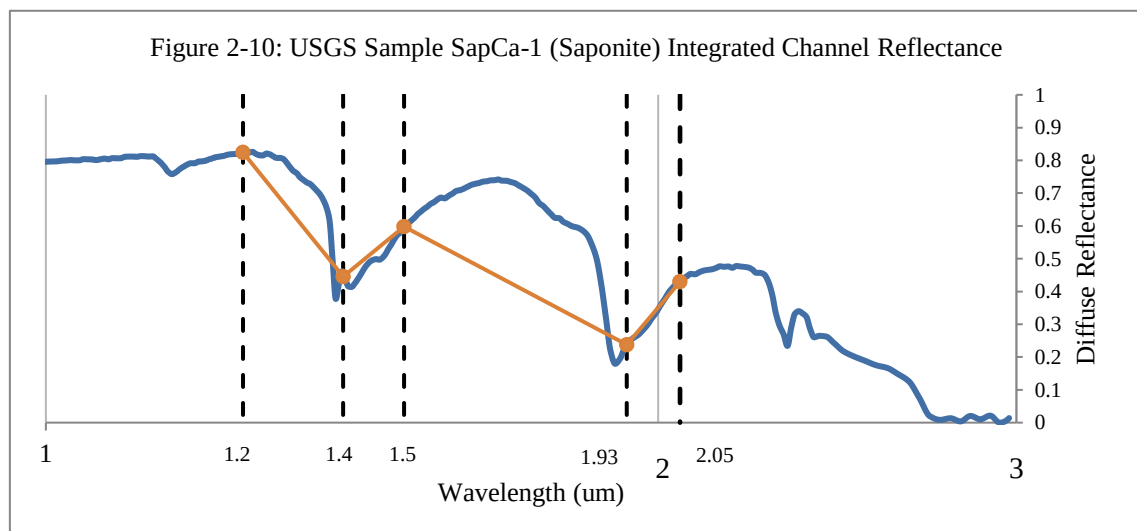
aqueous conditions (Evdokimova et al., 2009, Murchie et al., 2009, Thollot et al., 2012). In the simplest terms, hydrated minerals have bonded OH^- or H_2O (Rivkin et al., 2002). These produce spectral absorption features that can be used for diagnostics. In particular, bonded OH^- produces a strong absorption at $1.4\ \mu\text{m}$ (Thollot et al., 2012) while bonded H_2O and water ice produce a strong absorption at $1.93\ \mu\text{m}$ (Clark, 1981, Evdokimova et al., 2009, Thollot et al., 2012) (see Figure 4-22 for a representative water ice spectrum). These two frequencies, $1.4\ \mu\text{m}$ for bonded OH^- , and $1.93\ \mu\text{m}$ for H_2O ice, become the two principle absorption feature bands specific to this thesis.

Selection of anchor bands

When an anchor band is placed on either side of the absorption peak, there will be a concave shape with a negative ratio of the three bands that indicates a positive identification of the desired material. Here I selected $1.25\ \mu\text{m}$ and $1.5\ \mu\text{m}$ for use as the anchor bands around the $1.4\ \mu\text{m}$ absorption peak to detect bonded hydroxide. The $1.93\ \mu\text{m}$ absorption band for water ice is anchored by the $1.5\ \mu\text{m}$ band and a band centred at $2.05\ \mu\text{m}$. All of these choices were dependent upon available technology solutions described in Chapter 3 and the modelling confirmation in Chapters 4 and 5.

Saponite as an example of reflectance bands applied to a hydrated mineral

Figure 2-10 provides saponite as an example of the five reflectance bands applied to a mineral with both bonded OH^- and H_2O . The spectral absorption features are quite apparent, and the five bands are connected by a line that shows a concave depression around the $1.4\ \mu\text{m}$ and



1.93 μm bands. This can be interpreted as a positive indication of both hydroxide and water in this mineral. This would result in a positive identification of a hydrated mineral and a notation of how it is hydrated (e.g., hydrated with just bonded OH^- , just H_2O , or both). Ratios and/or differences of these five diagnostic bands should allow the determination of the presence and discrimination of water ice and hydrated minerals from non-hydrated minerals (Table 4-2).

2.7 Mixed minerals on Mars: Vertical and Horizontal Stratigraphy

Figure 2-5 identified a number of minerals that have been determined to be on the surface of Mars. Examples of these were collected and characterized for use in this thesis. Additional samples were identified for use in models in Figure 2-7. The last important detail is an assessment of the mixing ratios of these minerals. Which ones can and should be mixed and at what percentages. This analysis was made from a review of the available literature and cross-referenced against samples that are in the thesis sample set. Not all minerals are found together because co-location and mixing of minerals is dependent upon diagenesis of basic mafic minerals (such as basalts) and/or aeolian transport. Table 2-6 identifies which of these minerals have been found mixed on the surface of Mars.

Table 2-6 Mixed minerals found on Mars

Mineral	CaCO_3	Basalt	Gypsum	Halite	Jarosite	Quartz	Mont.	Hematite	Comments
CaCO_3									
Basalt	h								
Gypsum		g							REMS-GT sensor cal.
Halite									
Jarosite		h							
Quartz									
Mont.	d	e			c, e				General phyllosilicates
Hematite					d, f				
Olivine	a, b, d						d		
JSC Mars-1	h		d						Type II surface material

Table 2-6 References: a) Morris, et al., (2010), b) Ehlmann, et al., (2008), c) Farrand, et al., (2009), d) Murchie, et al., (2009), e) Ehlmann, et al., (2013), f) Squyres, et al., (2004), g) Martin-Redondo, et al., (2009), h) Based on general reading, basalt as a primary mineral and JSC Mars-1 as a general surface material would be reasonably common on the surface mixed with the other minerals.

Mixing ratios

Mixing of hydrated minerals, non-hydrated minerals, and water ice are suggested per the available literature from Mars data-sets and the stock of project minerals (Table 2-7). Gypsum was mixed with basalt as a calibration scheme for the RMS-GT sensor (Martin-Redondo et al., 2009), and is added to the test configurations.

Table 2-7 Proposed mineral mixing ratios for thesis models and testing

Mineral 1	Mineral 2	Mix Rates	Comments/References
Gypsum	Basalt	Basalt:Gypsum 100/100; 70/30; 50/50; 30/70 (by mass distribution)	Used to calibrate the RMS-GT sensor for MSL. Martin-Redondo, et al., (2009); however, according to mixing with sand, shouldn't be more than 40% gypsum. Squyres, et al. (2004), Murchie et al., (2009)
Gypsum	JSC Mars-1	Gypsum:JSC Mars-1 100/100; 70/30; 50/50; 30/70 (by mass distribution)	Gypsum dunes mixed with Type II surface material with a maximum gypsum:JSC Mars-1 mix of 35/65. Murchie, et al., (2009); Match calibration run by RMS-GT
Gypsum	Pyroxene	0-100% gypsum in 5% increments plus 1% and 99% gypsum.	Pyroxene is a common material on the Mars surface. It has a strong 2 μ m absorption band that could mask hydration bonds. Hapke model only as a worst case.
Water Ice	Basalt (light palagonite)	0-100% water in 5% increments plus 1% and 99% water.	Basalt is a material on the Mars surface. Testing revealed it as a weathered palagonite. Hapke model only.
Water Ice	Mars JSC-1 (dark palagonite)	0-100% water in 5% increments plus 1% and 99% water.	Mars JSC-1 (palagonite) was used as a proxy to dark materials on the surface for the Phoenix mission analysis of surface water ice composition. (Cull et al., 2010, Evdokimova et al., 2009). Hapke model only.
Water Ice	Pyroxene	0-100% water in 5% increments plus 1% and 99% water.	Same as gypsum:pyroxene models: Hapke model only as a worst case.

Vertical and horizontal Stratigraphy

Knowledge of the vertical and horizontal layering of the mineral layers is important in order to understand the duration of any specific process leading to the formation of a specific mineral. The thickness of the vertical layers is also important in order to determine the required accuracy of the sensor system to differentiate mixed layers. The spot size of the sensor is expected to be about 10 mm, so if pure minerals have thicknesses of 10-100's of metres and with sharp

boundaries in-between them, it is possible that it isn't as important to be able to discriminate mixed minerals from diagenesis. On the other hand, some minerals have significant mixing from Aeolian processes such as the gypsum sand dunes.

Table 2-8 provides available information on vertical and horizontal layering for minerals within the thesis sample set. While vertical thicknesses were found for some minerals, there is little information available. Vertical analysis was mostly from orbital observations, but these have very limited spatial resolution that is not sufficient to analyse thin bands. Gypsum and jarosite were determined from ground observations. Minerals formed from diagenesis should have much thicker bands than those from aeolian transport. For now, it is assumed that boundaries are sharp and discrete.

Table 2-8 Vertical and horizontal stratigraphy resolution

Mineral	Horizontal (m)	Vertical (m)	Comments/References
CaCO ₃	-	20	Murchie, et al., (2009)
Gypsum	100's	0.3 to 0.5	Gendrin, et al., (2005); Squyres, et al., (2004)
Jarosite	-	0.3 to 0.5	Squyres, et al., (2004)

2.7 Summary and Science Requirements Traceability

IR thermal emission and reflectance were selected as a means to the measurement of the Science Requirements (Table 1-4). A five-channel filter radiometer instrument was proposed. The five channels selected for this instrument are: 1.25 µm, 1.4 µm, 1.5 µm, 1.93 µm, and 2.05 µm. Performance specifications of the instrument must be specified for what the components (and integrated system) must meet in order to satisfy the Science Objectives.

The science requirements (Table 1-4) can be traced to the performance requirements through the traceability matrix shown in Table 2-9: science requirements to instrument performance traceability matrix. This matches the science objectives to specific observable and measureable signatures and then specifies spectral, radiometric, coverage, and sampling requirements and performance. The performance data of the tested components and instruments are presented in chapters 3 and 6.

Table 2-9: Science Requirements to Instrument Performance Traceability Matrix

Science Objective	Observable Signatures	Measurement Goals	Spectral and Radiometric			Coverage and Sampling
			Channels	Performance Requirements	Measured Performance	Requirements and Performance
1. Determination of Water Ice and/or Bonded water	Absorption Peak at 1.93 μm of reflected light	>5% water content	1.5 μm	High reflectance band with accuracy $\pm 10\%$	TBD	Requirements: TBD Performance: TBD
			1.93 μm	Absorption band with accuracy $\pm 10\%$	TBD	
			2.05 μm	High reflectance band with accuracy $\pm 10\%$	TBD	
2. Determination of Bonded OH ⁻	Absorption Peak at 1.4 μm of reflected light	Measurement of specific minerals: jarosite.	1.25 μm	High reflectance band with accuracy $\pm 10\%$	TBD	
			1.4 μm	Absorption band with accuracy $\pm 10\%$	TBD	
			1.5 μm	High reflectance band with accuracy $\pm 10\%$	TBD	
3. Determination of non-hydrated minerals	Flat spectral signature across water absorption peaks at 1.4 μm and 1.93 μm of reflected light	Measurement of specific minerals: basalt	Broadband IR detector (0.4 μm to 50 μm), with 5 Channel sources	IR wide passband 0.4 μm to 2.5 μm with >70% transmission; Source channels emitting at 1.25, 1.4, 1.5, 1.93, and 2.05 μm wavelengths.	TBD	
4. Determine temperature of subsurface environment	Emitted thermal flux	190-330K $\pm 3\text{K}$	Broadband IR detector (0.4 μm to 50 μm)	IR passband with accuracy <3K over 190-300K range.	TBD	
			Narrowband IR detector (25.2 $\mu\text{m} \pm 30 \text{ nm}$)	IR passband with accuracy <1K over 190-300K range.	TBD	
5. Determination of specific minerals found on Mars (Project Goal)	Shape and intensity of spectral curve across all channels of reflected light	Measurement of specific minerals: calcium carbonate, gypsum, jarosite, basalt	Broadband IR detector (0.4 μm to 50 μm), with 5 Channel sources	IR wide passband 0.4 μm to 2.5 μm with >70% transmission; Source channels emitting at 1.25, 1.4, 1.5, 1.93, and 2.05 μm wavelengths.	TBD	

Chapter 3: Component selection and testing

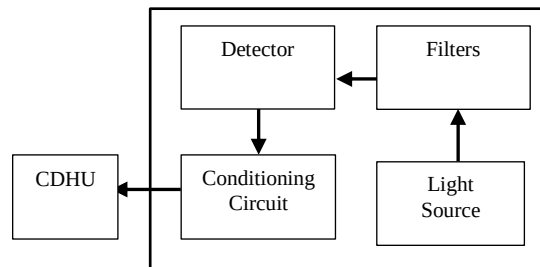
3.1 Introduction

The development of the integrated field instrument for the measurement of IR reflectance and IR thermal emission followed the process and steps as outlined in the flowchart in Figure 1-6. The following sections identify the critical path components; the criteria for selection and testing of a variety of available commercial off the shelf (COTS) components; and the final selection of components which met the performance requirements necessary to satisfy the science objectives (Table 1-4). Components were used in Chapters 4 and 5 to generate a theoretical performance model for an integrated instrument. Selected components were used to design and test instrument prototypes in Chapter 6.

3.2 Selection and Testing of Critical Path Components

The proposed combined thermal IR radiometer and IR reflectometer is a reasonable approach as the purpose of this device is not as a general survey instrument, but rather, to discriminate specific mineral types and/or

Figure 3-1: Borehole Radiometer Block Diagram



classes which have already been identified on the surface of Mars. There are seven major subsystems in the integrated instrument (Figure 3-1). These are described as follows:

- Detector: A device that can make a useful measurement of the radiation incident on the active element of the device.
- Filters: These are multi-layer interference filters that allow a specific frequency through to the active element. These will be determined by the specific scientific objective to be measured.
- IR Source: This is required for the IR reflectance measurement.
- Conditioning Circuit: Designed to amplify and condition the voltage generated by the detector above the various sources of noise.
- Command and Data Handling Unit (CDHU): A compact microcontroller.
- Thermal control: Temperature sensors, thermal heater, and a control circuitry.

- **Mechanical System:** The instrument support structure including internal structure and thermal control blocks, calibration surfaces, and exterior sheathing.

The detector, filters, and light source directly affect the integrated instrument performance. Proper selection and testing at the component level is necessary to ensure that integrated system performance will meet the science objectives.

3.3 Detector: Testing and Selection

Preliminary Selection Criteria and Manufacturers Data

The initial criteria for selection of detectors were driven by the size restrictions associated with the Icebite drill (Section 1.3). The expected diameter of the Icebite drill lead-string of ~25mm O.D. eliminated all but the simplest types of detectors. Additional criteria included uncooled, functional wavelength range, no mechanical chopper or other moving parts, commercially available, and flight heritage (when possible). This resulted in a short list of types of detectors that fell within the size limitations while meeting the preliminary performance specifications (Table 2-9). These included photovoltaic detectors, photoconductors, pyro-electrics, bolometers, and thermopiles.

The IR thermopile detector, in particular, responds to the temperature change at the junction of two different metals due to incident radiation absorbed at the junction, has a good detectivity, and does not need to be chopped if thermally stable. This causes the voltage generated by the junction to fluctuate (also the Seebeck effect) (Wolfe and Zissis, 1978).

A typical single element IR thermopile detector is shown in Figure 3-2 (Haenschke, 2012). This is a single element detector and is the same type that is used by the REMS-GTS on the Mars Curiosity Rover (Ramos et al., 2012). There are other versions that have 4, 8, and 16 active elements in a single package design.

A single element design was selected for this thesis in order to reduce space requirements. Detectors tested in this thesis were purchased from Dexter, Perkin Elmer, and IPHT



Fig 3-2: Single Element Detector

Jenna. These included the Dexter S25 with no window, with the 6.5 μm cut-on window, and with the KRS-5 window; the Perkin Elmer (PE) Surface Mount Device (SMD) thermopile; the Institute of Photonic Technology (IPHT) Jenna TS-72 with the window removed; and the IPHT TS-80 with the Si window (Table 3-1).

Except for the PE SMD, all others came in a T-05 can with a typical internal geometry shown in Figure 3-3. These have an active area element mounted within a gas back-filled volume and covered with a window. Typical Dexter window options are shown in Figure 3-4.

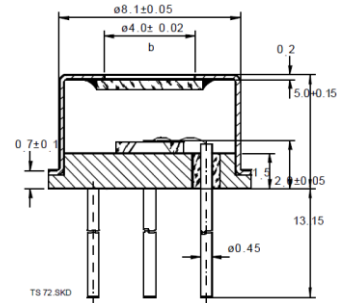
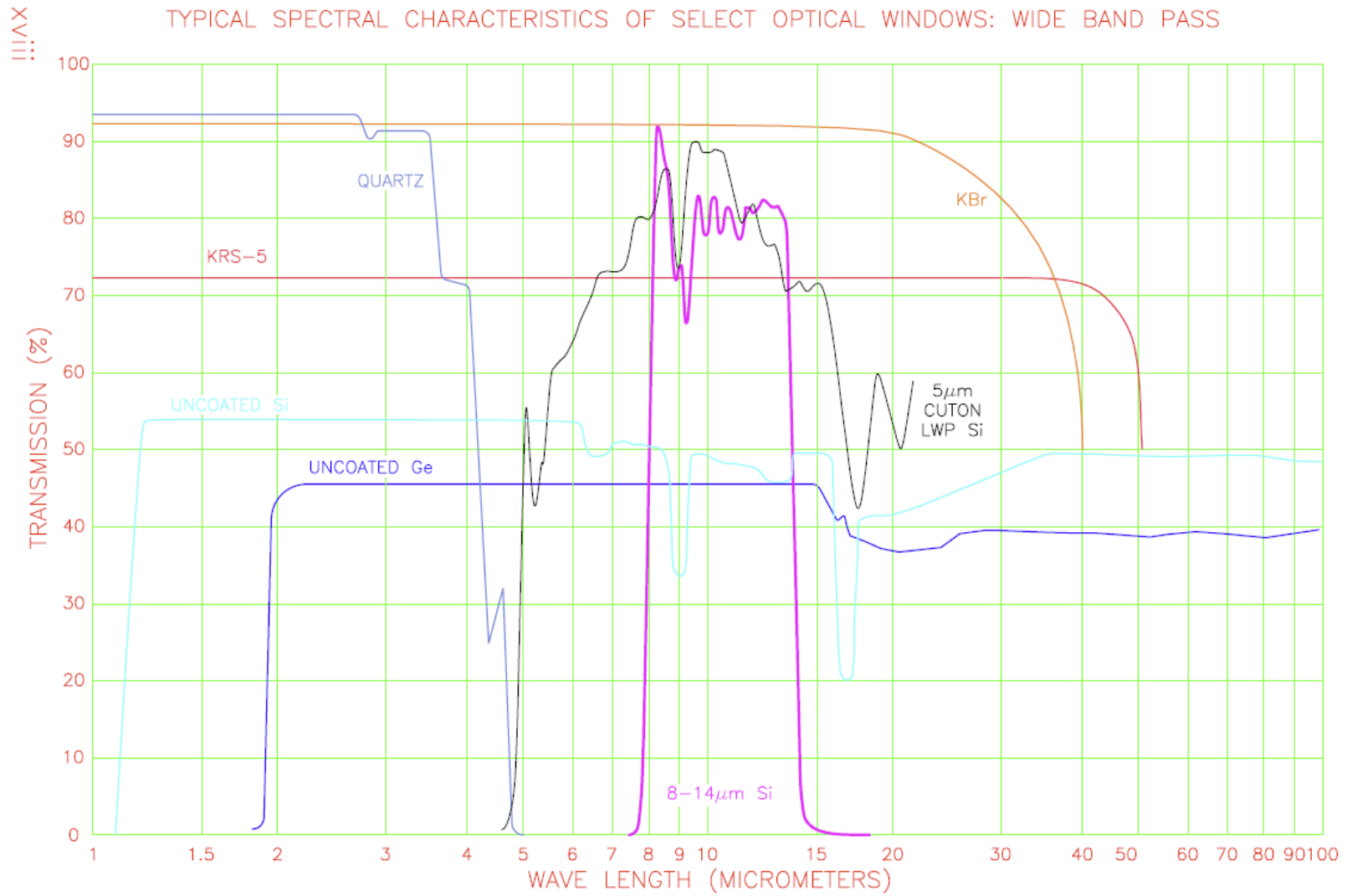


Fig 3-3: Internal Geometry Single Element Detector

There are a number of manufacturers specifications that provide an indication of the detector performance capabilities (Houghton and Smith, 1966, Sowen, 1971, Taylor, 2005, Wolfe and Zissis, 1978). These include:

- Responsivity: the ratio of the electrical output to the incident energy on the active area of the detector.
- Noise Equivalent Power (NEP): This power will produce a signal equal to the rms noise for a 1 s integration time. This varies with the square root of the area of the detector.
- D*: The values for detector performance vary with the design (including size and shape of the active area of the detector and the type of the materials used). R. C. Jones (1953) suggested this specification as a means to compare detectors. It is the reciprocal of the normalized NEP and can be calculated by dividing the square root of the active area of the detector by the NEP, with an integration time of 1s. This eliminates the size of the detector from the performance calculation to allow comparison of different detectors.
- Signal to Noise Ratio (SNR): This is the ratio of the useful signal and the background noise. Background noise includes the fluctuations in environmental thermal emission, detector noise, electrical noise of the conditioning circuit, and thermal noise due to changes in temperature of the detector.
- Window Spectral Transmission Range: The frequency transmission properties of the window of the detector (when present).
- Noise Equivalent Radiance (NER): The change in target radiance that changes the signal by an amount equal to the noise for the instrument, with an integration time of 1 s.

Figure 3-4: Dexter Window Spectral Characteristics



NOTE: Other Optical Windows and Filters available.
Please contact us for details.

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734-426-3921

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Table 3-1 provides a subset of the manufacturers' performance data for these sensors, when it was available. A principal concern was that the detectors are typically tested by the manufacturer

Table 3-1: Manufacturers' Performance Data for Thermopile Detectors Selected for Testing

Technical Parameter	Dexter S25 ^a	IPHT TS-80	IPHT TS-72	PE SMD
D* (10 ⁸ cm ² rtHz/W)	2.5	5.5	4.9	0.8
NEP (nW/rtHz)	0.10	-	-	-
SNR (rtHz)	2,062	-	-	-
Responsivity (V/W)	193.9	230	210	77
Noise Voltage (nV/rtHz)	19.4	≤ 20	≤ 20	42
Operating Temp (°C)	-50 to 100	-20 to 85	-20 to 85	-25 to 100
Window Type	KBr	Silicon	Silicon	None
Spectral Range (μm)	1 to 40	1 to 15	1 to 15	-
% Transmission	93	< 55	< 55	N/A

a) Manufactures data for Dexter S25 provided for device with a KBR window only

with a specific configuration of hardware (detector, window, gas-backfill, etc.) and under conditions and geometry which favorably optimize the results. Because the test protocols can vary significantly between manufacturers, each sensor was independently tested for this thesis in a common configuration in order to allow a direct comparison of performance.

Testing and selection of Thermopile Detectors

The primary test for the detectors was for the measurement of radiance. This allowed the determination of the NEP, the Noise Equivalent Radiance (NER), and the D*. From these values, along with the filter transmission specifications, additional calculations and plots can be made for SNR and Noise Equivalent Temperature (NET), as a function of the temperature of the material. A final set of calculations and plots can be made to compare the system performance in the expected final integrated instrument geometry to the NEP and NER.

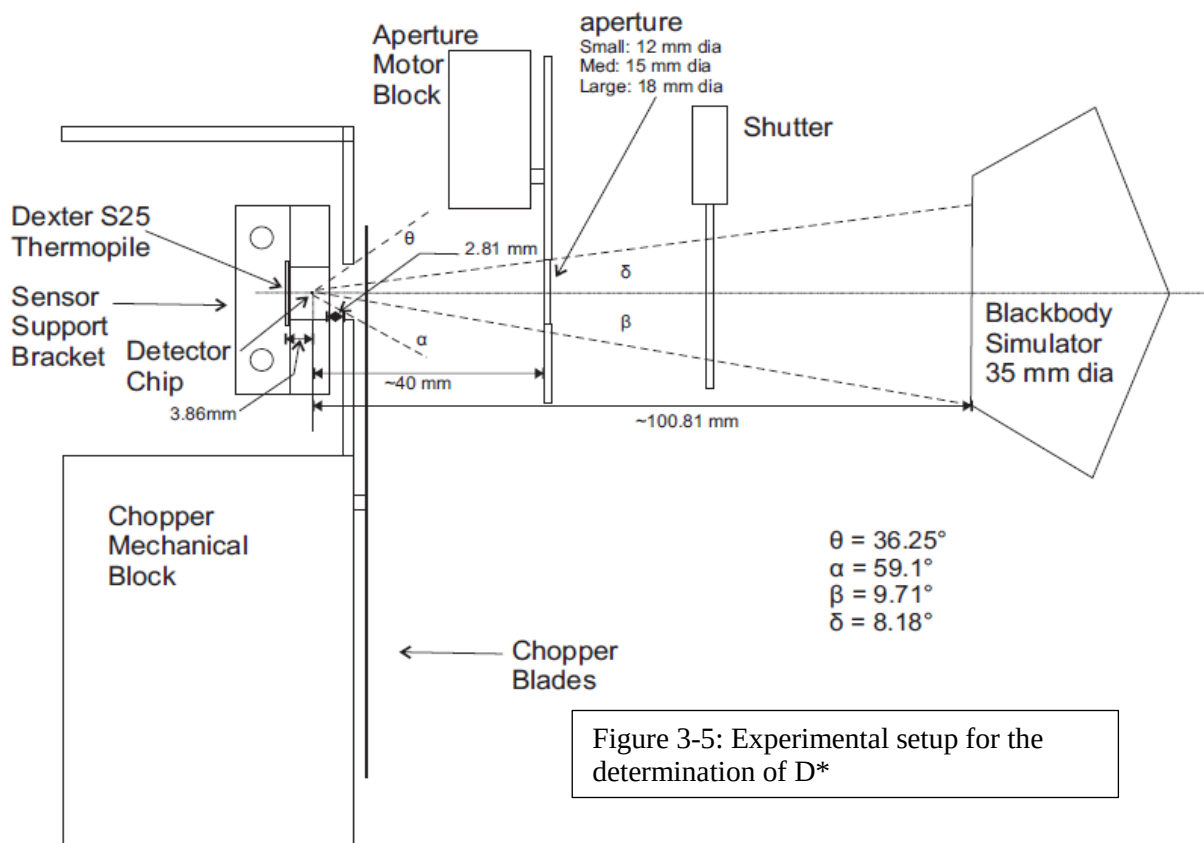
Method

A differential method was used in which the radiance and voltages generated from two temperatures are measured by the detector. Measurements were made in a vacuum chamber that was outfitted with a calibrated blackbody source, a chopper, a shutter to block the view to the blackbody, and a multi-aperture wheel to allow a change in the solid angle measured during the

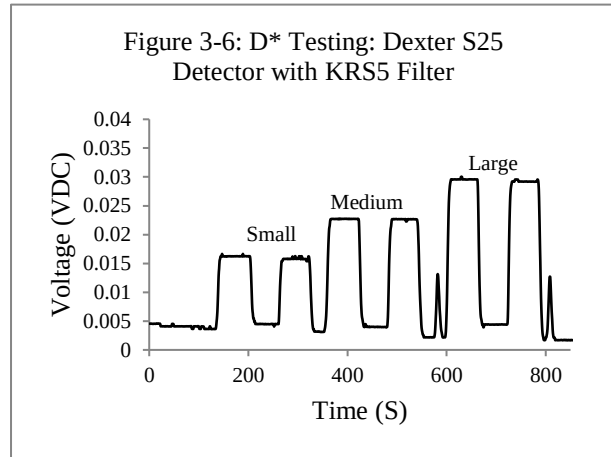
test. Figure 3-5 shows a typical set up with the sensor mounted on a support bracket behind the chopper.

The manufacturers' specifications for the internal sensor geometry (Figure 3-3) were used in addition to measurement of distances within the experiment block to allow the calculation of the distance from the front of the blackbody to the detector surface and the solid angle.

The solid angle is the view of the detector active surface to the blackbody surface. The full field of view (θ) of the detector active surface including physical limits from the aperture of the detector window (provided by the manufacturer) is the largest possible viewing angle. In this test configuration, the viewing angle is limited by the aperture on the chopper mechanical block (α), the size of the blackbody simulator (β), and the aperture of the aperture wheel (δ). The smallest of these denotes the actual scene viewed by the detector and is used to calculate the solid angle. The values for each angle are shown in Figure 3-5. The chopper frequency was set to ~ 21 Hz.



Once the vacuum chamber was evacuated to roughly 6.9×10^{-6} bar, two temperatures were measured with the detector. These were the blackbody simulator temperature set to 375 K and the shutter temperature at room temperature. The output signal from the detector was passed through the vacuum chamber to a Stanford Research Systems (SRS) pre-amplifier. The SRS pre-amp amplified the signal by 1,000x and conditioned it with low and high pass filters in order to reduce the out of band signal noise. This was then passed to an SRS830 lock-in amplifier that demodulated the detection of the blackbody signal by the elimination of the AC component from the chopper. This final conditioned signal was passed to a data-logger. The blackbody temperature was measured with each of the three sizes of the aperture wheel and included a measurement of the shutter temperature in-between each aperture measurement. This allowed the differential measurement of two temperatures, with a choice to use the values for any of the three aperture sizes in the calculations. An example of a typical fully conditioned output signal from this experiment is provided in Figure 3-6 with the three aperture sizes: small, medium, and large.



Calculations

Calculation of NET was according to Equation 3-1. The frequency was set to 396 cm^{-1} to represent the temperature channel of the instrument.

Eq: 3-1
$$NET = \frac{NER}{\frac{dB}{dT}}$$

K

Where dB/dT is the differentiated Planck function at each temperature

$$\frac{dB(\nu, T)}{\partial T} = \frac{C_1 C_2 \nu^4 \exp\left(\frac{C_2 \nu}{T}\right)}{T^2 \left[\exp\left(\frac{C_2 \nu}{T}\right) - 1 \right]^2}$$

Where:

$$C_1 = 1.1911 \times 10^{-8}$$

$$C_2 = 1.439$$

ν = wavenumber

T = Temperature

$$\text{Wm}^{-2}\text{sr}^{-1}(\text{cm}^{-1})^{-4}$$

$$\text{K}(\text{cm}^{-1})^{-1}$$

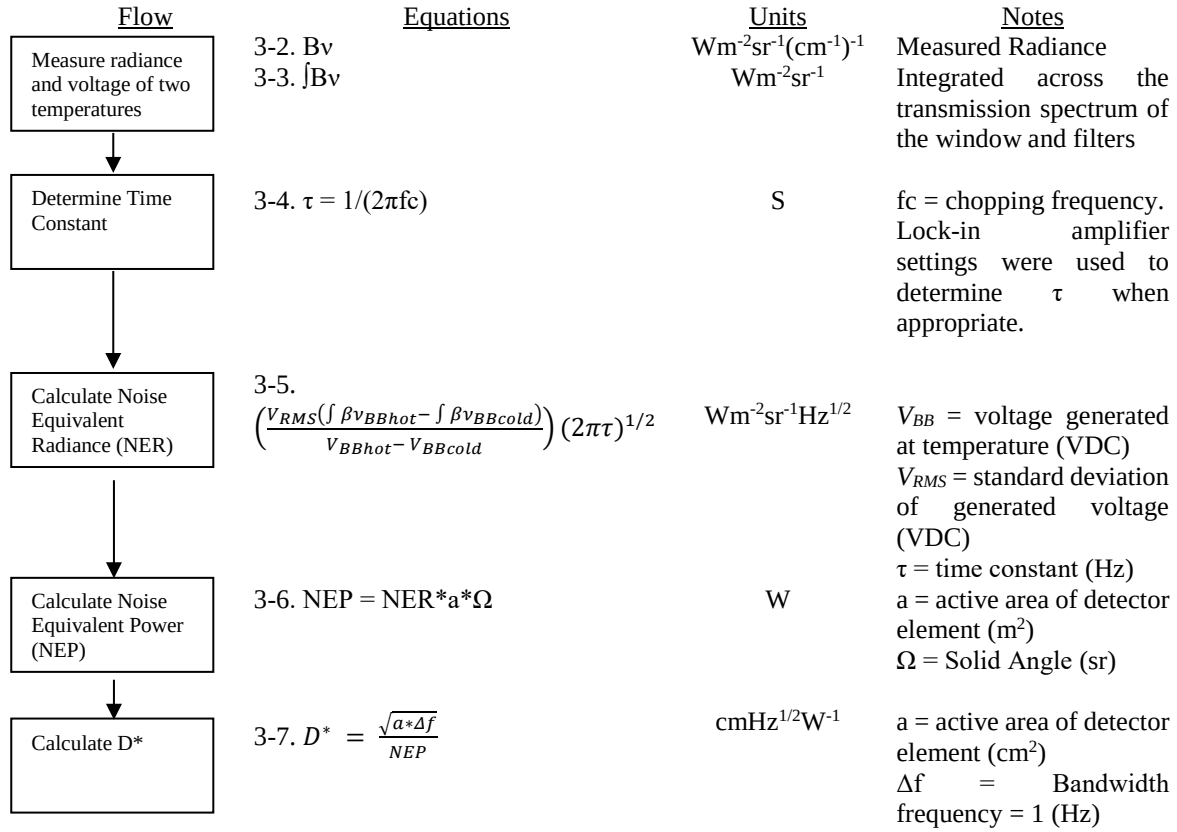
$$\text{cm}^{-1}$$

$$\text{K}$$

C1 and C2 are the first and second radiation constants (Houghton, 1997)

The collected data were used to calculate the values of NER, NEP, and D*. Figure 3-7 shows the method and equations 3-2 to 3-7 for each step necessary to calculate D*.

Figure 3-7: Flow Chart for the Measurement and Calculation of D*



Calculation of SNR was according to the Equation 3-8.

Eq: 3-8 $SNR = A \Omega D^* \left(\frac{\sqrt{\Delta t}}{\sqrt{a}} \right) \int L \Delta v$

Where:

A = area of detector	m^2	The value for $L \Delta v$ must be integrated across the spectral response range of the window/filter for each temperature.
Ω = solid angle	sr	
D^* = detectivity	$\text{cmHz}^{1/2}\text{W}^{-1}$	
Δt = integration time	s	
a = area of detector	cm^2	
L = measured radiance	$\text{Wm}^{-2}\text{sr}^{-1}(\text{cm}^{-1})^{-1}$	
Δv = frequency response range	cm^{-1}	

Results

The results of the testing and analysis for each of the sensors are provided in Table 3-2.

Discussion and sensor selection

The results of testing provided important information on the performance of the sensors necessary for the selection of one or more for use in this thesis.

Table 3-2: Sensor Performance Testing Results

Sensor	NER $\text{Wm}^{-2}\text{sr}^{-1}$	NEP $\text{nW/Hz}^{1/2}$	D* $\times 10^8 \text{ cmHz}^{1/2}\text{W}^{-1}$	SNR ¹ @ temperature	NET ¹ (K)
Dexter S25 w/6.5 μm window	0.084	0.036	6.95	247 @ 150 K to 8600 @ 300 K	NC ²
Dexter S25 with window removed	NR ³	NR	NR	NR	NR
Dexter S25 w/KRS-5 window	0.015	0.06	4.10	416 @ 150 K to 53,000 @ 300 K	0.09 to 0.006
PE SMD with no filter	0.258	0.00009	2620	NC	NC
PE SMD with 25.2 μm filter	NR	NR	NR	NR	NR
IPHT TS-72 window removed	NR	NR	NR	NR	NR
IPHT TS-80 with Si Window	0.164	0.15	3.89	33 @ 150 K to 43,000 @ 300 K	NC

1. Calculated for temperature range of 150 to 300 K; 2. NC – Not Calculated; 3. NR – No Result.

The Dexter S25 with the 6.5 μm filter had the best D* of $6.95 \times 10^8 \text{ cmHz}^{1/2}\text{W}^{-1}$ for the T-05 can configuration sensors as tested; however, the SNR was significantly lower than the same sensor as tested with the KRS-5 broad-band window. The Dexter S25 with the window removed had no result. This is attributed to damaging the detector during the removal of the window.

The Dexter S25 w/6.5 μm Long Wave Pass (LWP)-Si window performed well, but the spectral characteristics of the window (Figure 3-4) do not allow its use with any of the IR reflectance channels (e.g., 1.25, 1.4, 1.5, 1.93, 2.05 or 25.2 μm filters) which are all out of the performance range of this device (6.5- 20 μm). For this reason, the top was removed from one sensor in order to test it with the 25.2 μm filter, but the process of removal of the top likely damaged the sensor so that it was non-functional and produced no result.

The IPHT TS-72 sensor with the window removed also had no result. This could be attributed to a damaged sensor during the removal of the top or to degradation of the absorption coating due to exposure to air over a long period of time as it is not known when the top was removed (probably >4 years before the time of testing).

The PE SMD with no filter performed well, but when it was combined with the 25.2 μm filter, there was no result. This would indicate that the absorption coating on the sensor is not

responsive to that frequency range. Despite several requests, the manufacturer declined to send information regarding the frequency response of the sensor, so it had to be eliminated as an option.

The IPHT TS-80 with the Si Window also appears to function well, but the actual spectral transmission characteristics are unknown beyond what was indicated by the manufacturer data sheet of 1 to 15 μm with <55% transmission. This makes this sensor potentially useful for the 1.25, 1.5, and 1.93 μm filters, but not for the 25.2 μm filter. Further, the <55% transmission is an additional limitation as the Dexter KRS-5 window is closer to 73% transmission for a known range that covers all of the channels.

This summary indicates that the only potential sensor for development in this thesis is the Dexter S25 with the KRS-5 Window.

3.4 Filter Selection and Testing

A number of filters were purchased and tested (Table 3-3 and Figure 3-8 to 3-15). These were selected for testing according to the requirements set out in Table 2-9. Note: The 2.05 μm filter was ultimately not purchased and the manufacturers' data were used to calculate the models.

Temperature Channel A

Previously described in Section 2.5, a band pass centered around 400 cm^{-1} was determined in Figure 2-9 for the temperature channel. A filter from Reading University was identified which would potentially satisfy this requirement. This channel was specifically selected to optimize the measurement of temperature given an unknown sample on Mars.

Temperature Channel B

Also described in Section 2.5, Temperature Channel A was selected to make the measurement of temperature at a uniform point emissivity near 1 (Figure 2-9), a typical use of these types of sensors is to utilize a wide-band filter to measure the radiance across a larger frequency range to average out variations in emissivity. This is an approach that is currently being

applied by the Remote Environmental Monitoring Station (REMS) of GTS on MSL (Ramos et al., 2012, Sebastian et al., 2010). The approach for this channel is to utilize the Dexter S25 with the KRS-5 window with no additional filters installed.

Table 3-3: List of Filters Purchased and Tested

Channel (μm)	Manufacturer	Part #	Spectral Transmission Range (μm)	Description and Construction Type
1.25	Thorlabs	FB1250-10	CWL: 1250 nm ± 2 nm FWHM: 10 nm ± 2 nm Minimum Transmission: 40%	Double sandwiched glass substrate; Schott Borofloat & soda lime. Mounted in black anodized aluminum ring.
	Edmond Optics	NT65-773	CWL: 1250 nm ± 2 nm FWHM: 10 nm Minimum Transmission: >70% Blocking range: 200-1500 nm	Multiple sandwiched glass substrate, mounted in black anodized ring.
1.4	Thorlabs	FB1400-12	CWL: 1400 nm ± 2.4 nm FWHM: 12 nm ± 2.4 nm Minimum Transmission: 35%	Double sandwiched glass substrate; Schott Borofloat & soda lime. Mounted in black anodized aluminum ring.
1.5	Thorlabs	FB1500-12	CWL: 1500 nm ± 2.4 nm FWHM: 12 nm ± 2.4 nm Minimum Transmission: 35%	Double sandwiched glass substrate; Schott Borofloat & soda lime. Mounted in black anodized aluminum ring.
	Edmond Optics	NT65-778	CWL: 1500 nm ± 2.5 nm FWHM: 12 nm Minimum Transmission: >70% Blocking range: 200-1850 nm	Multiple sandwiched glass substrate, mounted in black anodized ring.
1.93	Spectragon	NB-1930-10	CWL: 1929.8 nm ± 10 nm HWHM: 9.4 nm Minimum Transmission: >70% Blocking: 3500 nm	Glass
2.05	Northumbrian Optical	SNB-2052-000311	CWL: 2052 nm BW: 27 nm Minimum Transmission: 54.7% Blocking: 3500 nm	Fused Quartz
25.2	University of Reading	SMCR 03124 CFV	CWL: 25200 nm HWHM: 1700 nm Minimum Transmission: 75%	Germanium substrate

Water Ice and Hydrated Minerals

As discussed in Section 2.6, two channels were identified for the detection and characterization of water ice and hydrated minerals; these were the 1.93 μm and 1.4 μm, respectively. There were combined with anchor bands at 1.25, 1.5, and 2.05 μm.

Testing and Characterization of Transmission Properties of Filters

The transmission characteristics of the purchased filters were tested with a Brüker IFS66v spectrometer. Measurements were made for the 1.25, 1.4, 1.5, 1.93 and 25.2 μm filters. The 2.05 μm filter was not purchased, so the manufacturers' data were used for calculations and models.

The spectrometer was set as follows: Beam splitter: KBr; Source: Globar; Detector Setting: FIR DTGS (Deuterated Tri Glycine Sulfate); Aperture: 5 mm; Scanner Velocity: 1.6 kHz; Sample Signal Gain: 1; Switch Gain: Off; Number of Scans: 300; Background: 50 scans. A background reading was taken before the measurement of the filter. The filters were then mounted on a bracket and centered in the measurement compartment of the spectrometer and measured individually. Measured spectra were interpolated to whole wave number values.

The transmission characteristics for the tested filters are provided in Figures 3-8 to 3-15. The spectral performance of the filters as tested indicated that the 1.25 μm (Figure 3-8) and 1.5 μm (Figure 3-9) filters from Edmond optics had a large spectral leakage band. The multilayer construction made these not suitable for use in this project because the filters are too thick for the tight borehole dimensions. The Thorlabs filters for 1.25 μm (Figure 3-10) and 1.4 μm (Figure 3-11) were excellent with low, out of range leakage. The Thorlabs 1.5 μm filter (Figure 3-12) also had significant leakage, but it was a smaller construction package than the Edmond Optics 1.5 μm filter; therefore, more suitable for this project. It must be matched against the IR source to determine if the spectral range of these overlap while excluding the leakage range (see section 3.6 for this analysis). The Spectragon 1.93 μm filter (Figure 3-13) was excellent with no leakage in the range of the LED source. The Reading 25.2 μm filter (Figure 3-14) was excellent with no leakage in the tested range. The Northumbrian Optical 2.05 μm filter (Figure 3-15) was not tested and data were based on the manufacturers' datasheet. Any thermal leakage in any of the channels can be eliminated with additional blocking filters or electronically chopping the signal.

Figure 3-8: Transmission characteristics
Edmond Optics 1250 nm filter

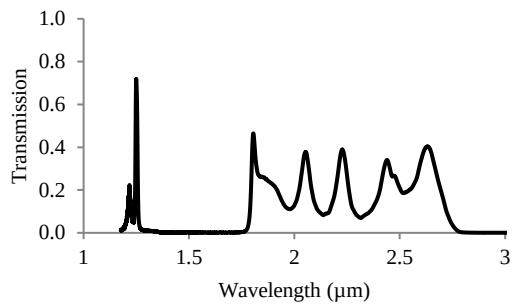


Figure 3-9: Transmission characteristics
Edmond Optics 1500 nm filter

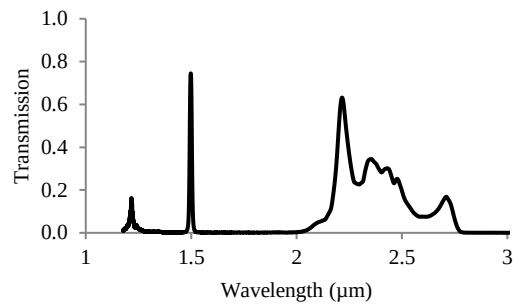


Figure 3-10: Transmission
characteristics Thorlabs 1250 nm filter

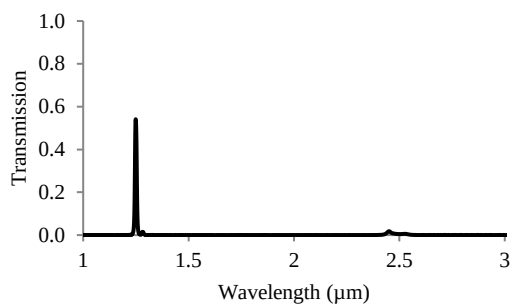


Figure 3-11: Transmission
characteristics Thorlabs 1400 nm filter

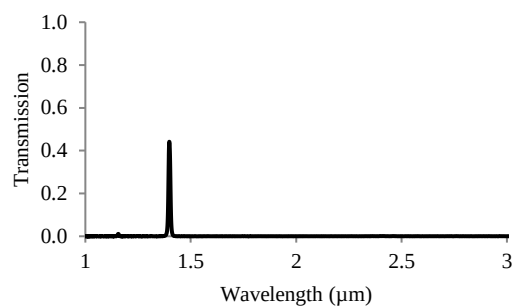


Figure 3-12: Transmission
characteristics Thorlabs 1500 nm filter

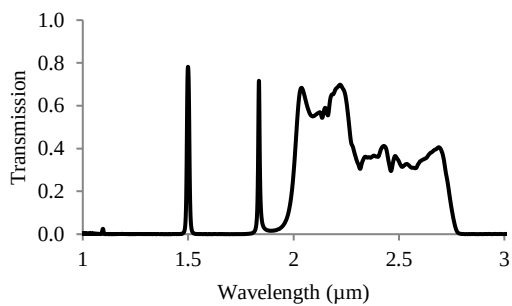


Figure 3-13: Transmission
characteristics Spectragon 1930 nm
filter

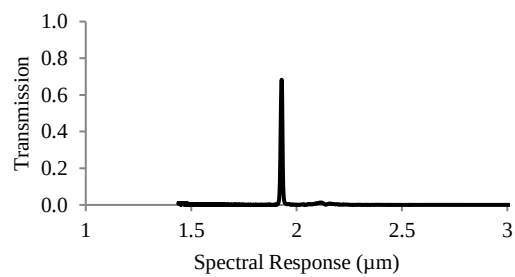


Figure 3-14: Transmission
characteristics Reading 25.2 μm filter

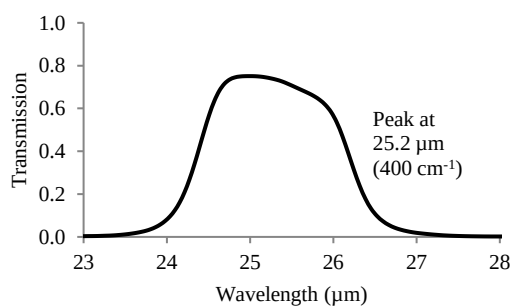
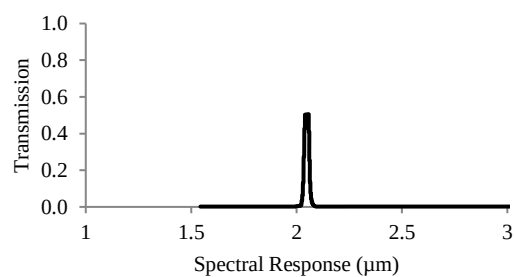


Figure 3-15: Transmission
characteristics Northumbrian 2050 nm
filter



3.5 Infrared Source Selection and Calculations

Borehole IR source requirements, limitations, and available solutions

IR reflectance radiometry requires a source of IR radiation. This is reflected off the surface and impinges on the detector that is recorded as a voltage. In the case of satellite and surface based instruments, the Sun serves as this source of IR radiation; however, a borehole instrument will require an artificial IR source. There are a few technical solutions that can provide this IR radiation, but most are limited by the size and power constraints.

Base Requirements

The most important requirement for the selection of an IR source is that it provides stable luminosity in the frequency range required by each of the channels (Table 2-9). Stable luminosity also avoids leaks from the filters. Short-term oscillation due to variations of the source itself or due to external factors like temperature variations have to be limited in order to ensure that the total instrument error is still within the original specifications. Some variation from the source is expected, but this must be managed. Variations are also related to long-term drift and degradation because the materials will break down from use or just post-manufacturing. Closely followed by this requirement are the constraints on size. The IR source would preferably be placed within the borehole instrument; however, there are options, for instance, to use a collimated source placed on the lander/rover with a fiber-optic feed down the instrument string that should be considered. The final consideration is the power consumption of the IR source. While this is not a hard requirement, a low power device is preferred.

Potential Options

There are two potential methods for an IR source: 1) blackbody emitter and 2) quantum emitter. Discussed in more detail in Section 1.7, any material with a temperature greater than absolute zero will emit blackbody radiation in the form of photons in the IR frequency range. This allows the measurement of surface temperature in the thermal channels, but can also be used to build an IR source for the reflectance channels. Common types of these are an incandescent lamp with a tungsten filament or a tungsten halogen light source. These are broadband devices and will

emit a spectrum of light from about near visible (~ 300 nm) to >5 μm , dependent upon their heated temperature (see Planck Function, Equation 1-1), and casing material transmission characteristics. These are typically high power devices that generate a lot of heat. They are required to be stabilized to ensure that the peak frequency doesn't shift with the change in temperature of the element. In terms of a Mars application, the source would have to be located at the surface and the light would be fed down through the lead-string to the measurement site.

Quantum emitters include both laser diodes and IR Light Emitting Diodes (LEDs). They generate photons by the recombination of electrons and holes across a semiconductor bandgap (Elias, 2008). The energy of the photon is equal to the difference between the recombined electron-hole pair such that the wavelength is determined by the type of material the diode is fabricated from. LEDs can have a narrow or wideband emission spectral range while laser diodes can be extremely narrow. Both are compact devices that are stable over time and have good optical power output levels. While the narrow bands of the laser diodes matches well to the channels, there are limited frequency ranges commercially available. LEDs, on the other hand, have wider bandwidths but have many more commercially available frequency ranges available. A comparison of each of the types is provided in Table 3-4 (data from Thorlabs). The LEDs are the preferred solution due to the commercially availability and frequency response range.

Table 3-4: Comparison of IR Source Options

IR Source	Output Frequency FWHM (wn)	Compact Dia x Length (mm)	Power Usage (W)	Short-term Luminal Stability (%)	Lifetime (Hrs)	Forward Optical Power (mW)	Commercially Available in Channel Range
Incandescent Lamp (tungsten)	22222 - 1818	16x10	7.2	1	5,000	100	Yes
Laser Diode	10	6x4	0.3	1	$>100,000$	150	Limited
LED	100-200	9x5	0.12	1	$>10,000$	2.5 - 25	Yes

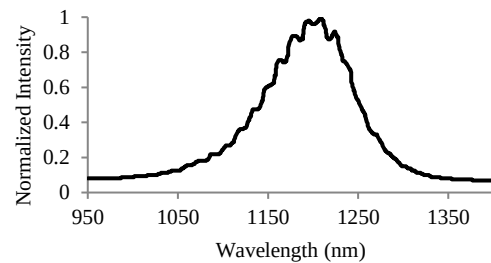
Selection of IR LED sources

A number of manufacturers were reviewed for potential IR LED sources. Specific components were identified to meet the science and engineering requirements and purchased (Table 3-5). These were modeled using the manufacturers' available data in order to determine the expected performance. This data will be used in the integrated models in Chapter 5.

LED Spectral Radiance Calculations

In order to develop predictive models of the performance of the integrated system, the amount of energy emitted by the LED has to be calculated. This value is typically measured with a PM120 type instrument which measures the total integrated power emitted by the LED in all forward angles and

Figure 3-16: Thorlabs LED 1200E
Spectral Intensity Distribution
Manufacturers Data, Doc: 16389-S01
Rev. A, 02/07/2007



is reported by the manufacturer as the forward optical power (Table 3-5) (Thorlabs datasheet). But this energy is distributed across a range of wavelengths as shown in Figure 3-16, which is an example of a typical spectral distribution for an LED.

Table 3-5: List of LEDs purchased and modeled

Channel (μm)	Manufacturer	Part #	Spectral Transmission Range (μm)	Description and Construction Type
1.25	Thorlabs	LED 1200E	CWL: 1200 nm ± 50 nm FWHM: 100 nm Half Viewing Angle: 15° ± 2° Forward Optical Power: 2.5 mW @ 20 mA	Heterostructures grown on InGaAsP substrate, encapsulated in round clear epoxy casing.
1.4	Hamamatsu	L10660-01	CWL: 1450 nm ± 50 nm FWHM: 120 nm Half Viewing Angle: 10° Forward Optical Power: 2.4 mW @ 50 mA	InGaAs substrate, encapsulated in a TO-46 can with a glass lens window.
1.5	Thorlabs	LED 1550E	CWL: 1500 nm ± 50 nm FWHM: 100 nm Half Viewing Angle: 15° Forward Optical Power: 1.2 mW @ 20 mA Total Optical Power: 2.0 mW @ 20 mA	Heterostructures grown on InGaAsP substrate, encapsulated in round clear epoxy casing.
1.93	Deep Red Technologies	LED19	CWL: 1950 nm ± 30 nm FWHM: 150 nm Half Viewing Angle: 30° Forward Optical Power: 1.0 mW @ 200 mA (Quasi-CW) Total Optical Power: 25.0 mW @ 1 A (pulsed)	Heterostructures grown on GaSb substrates, encapsulated in a TO-46 can with a clear glass window.
2.05	Deep Red Technologies	LED20	CWL: 2050 nm ± 50 nm FWHM: 200 nm Half Viewing Angle: 30° Forward Optical Power: 1.1 mW @ 200 mA (Quasi-CW) Total Optical Power: 28.0 mW @ 1 A (pulsed)	Heterostructures grown on GaSb substrates, encapsulated in a TO-46 can with a clear glass window.

The conversion to spectral power distribution by wave number assumes that the highest normalized intensity (~ 1 in Figure 3-16 as an example using the Thorlabs 1200E LED) is equal to the highest energy emitted in any single wave number parcel such that all others will be their normalized intensity times this value. The sum of all of these will be equal to the integrated forward optical power. Multiplying the normalized intensity of each wavelength by this maximum value results in the spectral power distribution by wavelength.

The area of the spot illuminated by the LED is dependent upon how far that the LED is set from the illuminated surface. Because the energy reaching the surface is attenuated by distance (inverse square of the distance), the radial intensity distribution must also be taken into account. For the purposes of an early assessment of the viability of this system and modeling, it was assumed that the LED would be 4 mm from the illuminated surface. As an example for the Thorlabs 1200E LED (Figure 3-17B), the angle of the cone of the light is the 20° as noted for the maximum of the radial intensity distribution (given in m^2).

Figures 3-17 A and B: Typical LED intensity distribution characteristics (Thorlabs 1200E)

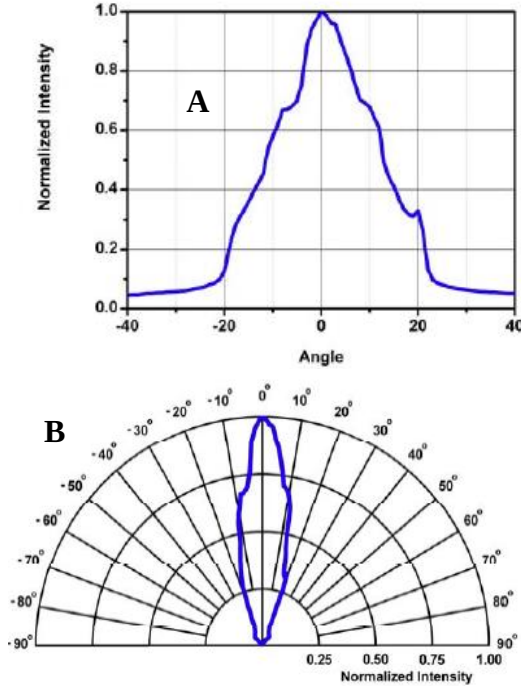


Figure 3-18: LED spectral power distribution Thorlabs 1200 nm LED

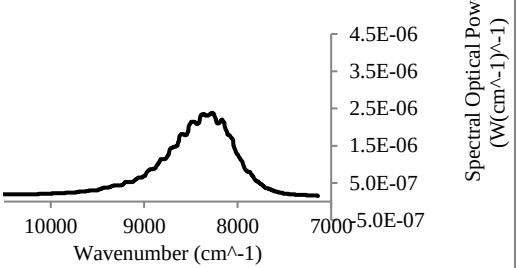


Figure 3-19: LED spectral power distribution Hamamatsu 1450 nm LED

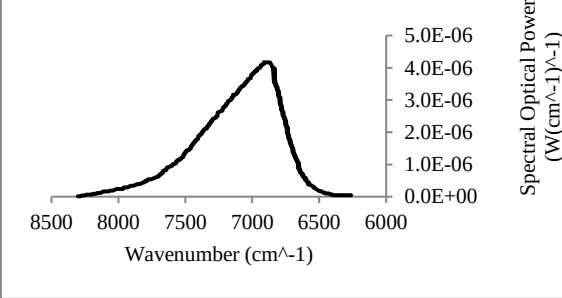
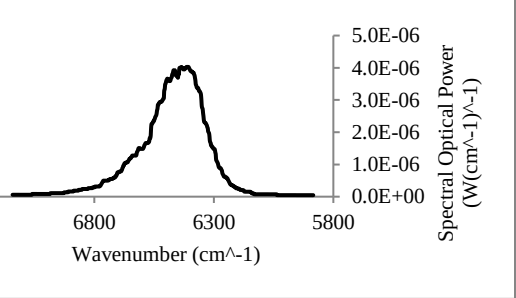
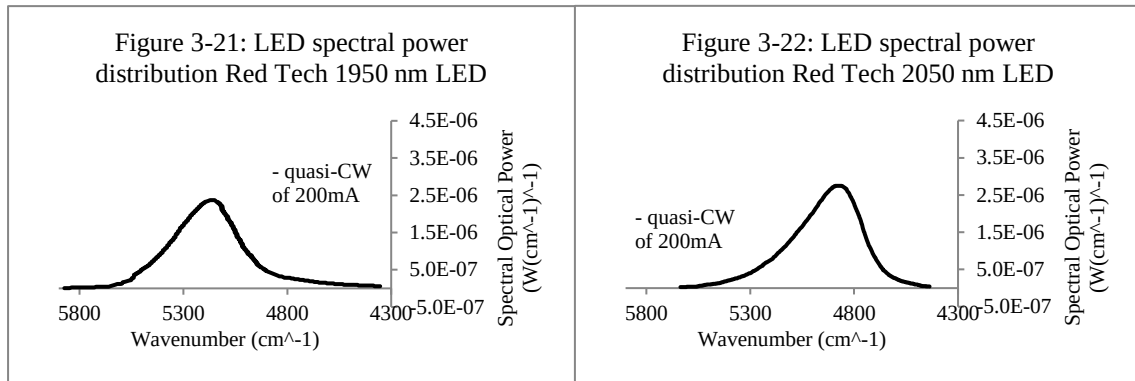


Figure 3-20: LED spectral power distribution Thorlabs 1550 nm LED

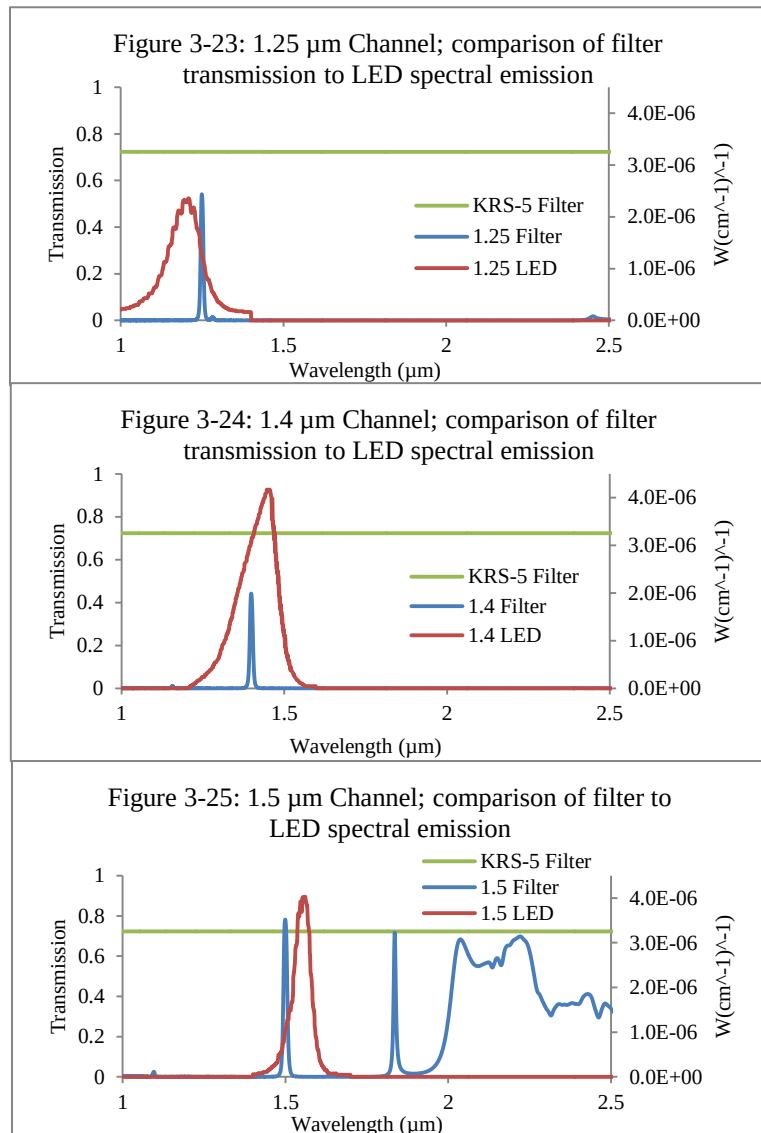


The results of the calculations for spectral power distribution are provided in Figures 3-18 to 3-22 for each of the 5 LEDs.

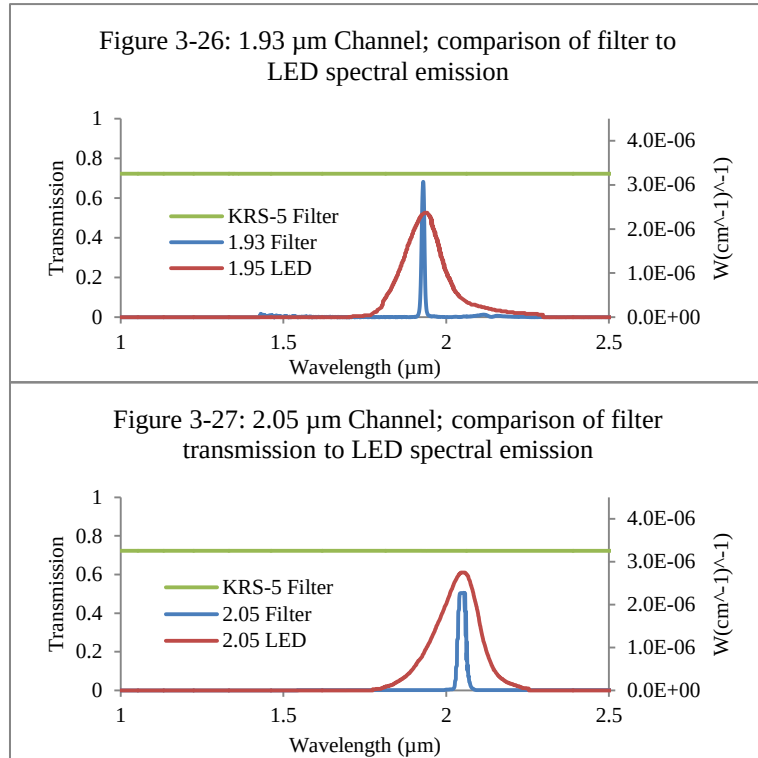


3.6 Analysis of Combined Filter and LED Pairs

In the reflectance channels of the filter radiometer design, the filter must be matched to an LED. If these are correctly matched, only the energy in the band of interest will be passed through to the detector. For this to work properly, there should be an overlap of the filter/LED pair with no leakage around the specific band of interest. As a sanity check on the components matched for each channel, these pairs are graphed in Figures 3-23 to 3-27.



From the figures, it can be seen that the 1.93 μm (Figure 3-26) and the 2.05 μm (Figure 3-27) are in very good alignment of the LED to filter peaks. This is important to maximize the amount of energy that is reaching the detector. The 1.25 μm (Figure 3-23) and 1.4 μm (Figure 3-24) channels have a minor offset, while the 1.5 μm



channel (Figure 3-25) has a significant off-set of the peaks. By missing these peaks, there is just less energy available at the detector. This will decrease the signal to noise ratio. This was tested as an integrated combination to determine the impact on the performance of the instrument in these channels. This data are presented in the integrated models in Chapter 5 and the bench top testing of the integrated prototypes in Chapter 6.

An additional concern in the 1.5 μm channel was that there are significant leaks in the filter transmission at about 1.8 μm and from 2 – 2.8 μm ; however, the LED is the source of the reflected energy which does not overlap with any of the leakage bands. Electronic chopping of the signal would also eliminate any thermal leakage. Finally, the peak luminosity is temperature dependent. LED temperature stability errors are discussed in Section 5.7 (Figure 5-27).

3.7 Summary of Selected Components

Specific components that satisfy the science requirements of Table 1-4, while meeting the engineering design limitations associated with a borehole configuration and COTS availability, are provided in Table 3-6: IR thermal emission channels, and Table 3-7: IR

reflectance channels. These were tested and/or evaluated and shown to meet the requirements on an individual component bases and as filter/LED pairs.

Table 3-6: IR Thermal Emission Channels

Band		
Diagnostic	Channel A	Channel B
Detector	Dexter S25 w/KRS-5 Window	Dexter S25 w/KRS-5 Window
Filter Source	25.2±1.7 µm University of Reading	None
LED Source	None	None

Table 3-7: IR Reflectance Channels

Band	1.25 µm	1.4 µm	1.5 µm	1.93 µm	2.05 µm
Diagnostic	H ₂ O Ice and Anchor	Hydrated Minerals (OH ⁻ band)	H ₂ O Ice and Anchor	H ₂ O Ice and Hydrated Minerals	Anchor
Detector	Dexter S25 w/KRS-5 Window	Dexter S25 w/KRS-5 Window	Dexter S25 w/KRS-5 Window	Dexter S25 w/KRS-5 Window	Dexter S25 w/KRS-5 Window
Filter Source	1250±10 nm Thorlabs, FB1250-10	1400±12 nm Thorlabs, FB1400-12	1500±12 nm Thorlabs, FB1500-12	1930±10 nm Spectragon	2052±27 nm Northumbrian Optical, SNB-2052
LED Source	1.20 µm Thorlabs, LED1200E	1.45 µm Hamamatsu L10660-1	1.55 µm Thorlabs, LED1550E	1.95 µm Deep Red Technologies	2.05 µm Deep Red Technologies

3.8 Summary, Update to Traceability Matrix, and Recommendations

The science requirements to instrument performance traceability matrix was previously presented in Table 2-9. As a result of the investigation and testing of components in this chapter, additional information is provided as an update to the traceability matrix and presented in Table 3-8. Primary changes are in reference to the selected Dexter S25 thermopile, its performance, and geometry (all taken from the manufacturers' data sheet).

The next step was to generate theoretical performance calculations using the data for these components and the data for the minerals collected as described in Chapter 2. These models formed the bulk of Chapters 4 and 5 and were used to confirm the validity of these choices as well as to confirm a bench-top testing configuration for an integrated instrument (Chapter 6).

Table 3-8: Science requirements to instrument performance traceability matrix (revised for chapter 3)

Science Objective	Observable Signatures	Measurement Goals	Spectral and Radiometric			Coverage and Sampling Requirements and Performance
			Channels	Performance Requirements	Measured Performance	
1. Determination of Water Ice and/or Bonded water	Absorption Peak at 1.93 μm of reflected light	>5% water content	1.5 μm	High reflectance band with accuracy $\pm 10\%$	TBD	Req: 38° unobstructed FOV of surface; Spot size 17 mm dia. @ 11 mm from detector chip; Vertical resolution 17 mm; Integration time <30 s. Perf: TBD
			1.93 μm	Absorption band with accuracy $\pm 10\%$	TBD	
			2.05 μm	High reflectance band with accuracy $\pm 10\%$	TBD	
2. Determination of Bonded OH	Absorption Peak at 1.4 μm of reflected light	Measurement of specific minerals: jarosite.	1.25 μm	High reflectance band with accuracy $\pm 10\%$	TBD	
			1.4 μm	Absorption band with accuracy $\pm 10\%$	TBD	
			1.5 μm	High reflectance band with accuracy $\pm 10\%$	TBD	
3. Determination of non-hydrated minerals	Flat spectral signature across water absorption peaks at 1.4 μm and 1.93 μm of reflected light	Measurement of specific minerals: basalt	Broadband IR Thermopile (0.4 μm to 50 μm), with 5 Channel LED sources	Thermopile IR wide passband 0.4 μm to 2.5 μm with >70% transmission; LED channels emitting at 1.25, 1.4, 1.5, 1.93, and 2.05 μm wavelengths.	Thermopile frequency response range 0.4 to 50 μm with >72% transmission. LEDs cover required bands.	
4. Determine temperature of subsurface environment	Emitted thermal flux	190-330 K $\pm$ 3 K	Broadband IR Thermopile (0.4 μm to 50 μm)	Thermopile IR passband with accuracy <3 K over 190-300 K range.	TBD	
			Narrowband IR Thermopile (25.2 μm $\pm$ 30 nm)	Thermopile IR passband with accuracy <1 K over 190-300 K range.	TBD	
5. Determination of specific minerals found on Mars (Project Goal)	Shape and intensity of spectral curve across all channels of reflected light	Measurement of specific minerals: calcium carbonate, gypsum, jarosite, basalt	Broadband IR Thermopile (0.4 μm to 50 μm), with 5 Channel LED sources	Thermopile IR wide passband 0.4 μm to 2.5 μm with >70% transmission; LED channels emitting at 1.25, 1.4, 1.5, 1.93, and 2.05 μm wavelengths.	Thermopile frequency response range 0.4 to 50 μm with >72% transmission. LEDs cover required bands.	

Chapter 4: Theoretical Performance Models

4.1 Introduction

The objective of this chapter was to develop thermal IR emission and IR reflectance models utilizing the underlying physics. These were developed to demonstrate the capability of the proposed methods to measure temperature and to detect and discriminate water ice and hydrated minerals mixed in a non-hydrated mineral matrix. Section 1.7 provided an overview of the fundamental IR thermal emission and IR reflectance theory.

A number of numerical performance models were identified in Section 1.8 that allowed the characterization of the theoretical performance of the instrument. These included a model for thermal channels A and B, reflectance models with linear and non-linear mixing of samples, and integrated system models for thermal and reflectance channels.

Data from the mineral spectra (Chapter 2) and component specifications (Chapter 3) were used to develop each of the models identified in Section 1.8. Single minerals were used to confirm the reflectance model methods in Section 4.3 while synthetic mixed minerals were used for the calculation of linear (Section 4.4) and non-linear Hapke models (Sections 4.5 to 4.8). Finally, The Hapke model calculated spectra are compared to measured results for a mixture of Basalt and Gypsum (Section 4.9). Integrated system models are presented in Chapter 5.

4.2 Thermal models and results

Two thermal channels were specified for this instrument (Table 3-6). Channel A includes a narrowband filter manufactured by Reading University (Figure 3-14) with a range of 364 to 424 cm^{-1} , centred at $\sim 400 \text{ cm}^{-1}$ (25.2 μm). Channel B includes the wideband KRS-5 window from the Dexter S25 detector (Figure 3-2). This has a spectral range from near VIS-IR to about 50 μm with a transmission of ~ 0.72 . The variation in the mineral emissivity in the frequency range of each channel leads to temperature measurement errors that must be quantified in the thermal model. This model provides an assessment of the method without consideration of the detector

performance. Integrated system models in Chapter 5 will consider all components in order to determine the predicted performance and errors.

Methods

Theory

The measurable energy emitted corresponds to the area under the curve bounded by the material emissivity and the filter/window transmission range. This varies with temperature, so must be calculated at each discrete temperature. The integrated channel radiance was calculated with equation 4-1:

$$\text{Integrated channel Radiance} = \int_{\nu_l}^{\nu_u} L(\nu, T) * M(\nu) * W(\nu) * F(\nu) d\nu \quad \text{Equation 4-1}$$

Where ν_l and ν_u are the lower and upper frequencies of the range; $L(\nu, T)$ is the Planck function radiance at the discrete temperature and frequency; $M(\nu)$ is the mineral emissivity spectrum; $W(\nu)$ is the window transmission characteristics; and $F(\nu)$ is the filter transmission characteristics.

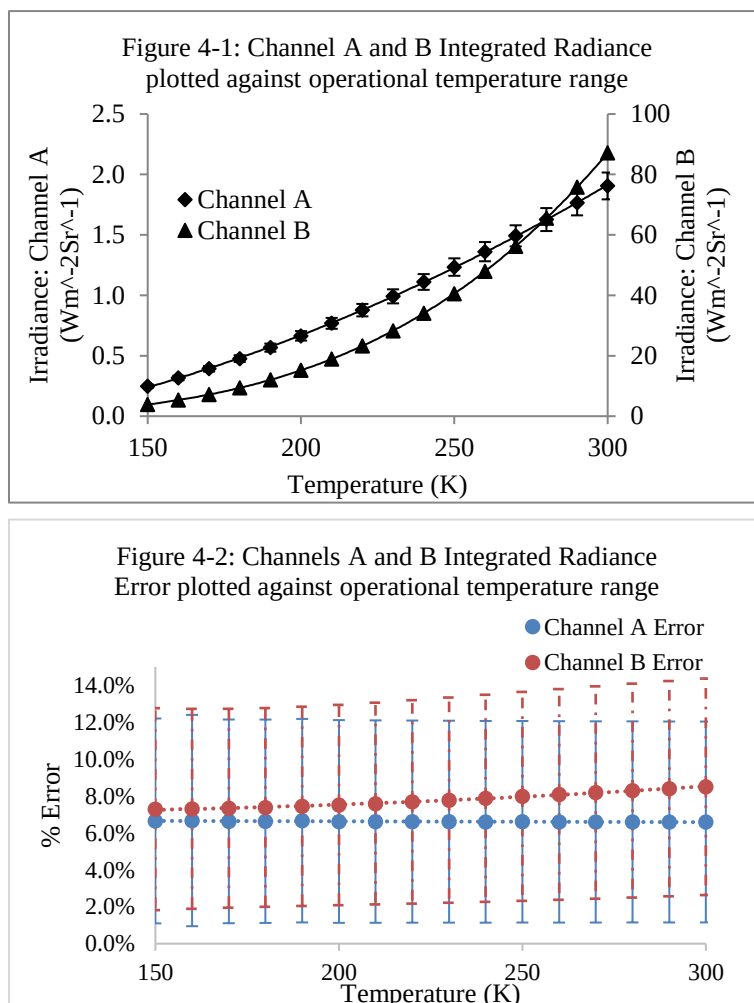
The emissivity of the materials was assuming (1 – Reflectance) as measured by RELAB. This was interpolated to 1 wave number intervals. The measured filter/window transmission range (Figure 3-14 and 3-4) were also interpolated to 1 wave number intervals. The Planck function at 10 K intervals from 150 to 300 K were calculated at 1 wave number intervals. The filter transmission is only included in the Channel A configuration. The integrated channel radiance was calculated for the average mineral emissivity for the 13 minerals listed in Table 2-4 within the frequency range for channels A and B.

Error calculations

To determine the extent of the errors, an estimate of the emitted radiance was generated for the average emissivity in the frequency range of the two channels within the temperature range of 150 – 300 K. The error is the difference between the calibration target radiance (assuming an emissivity = 1) and the average mineral radiance.

Results

The integrated channel radiance for the temperature range is plotted in Figure 4-1 for Channels A and B. The errors for each channel by temperature are plotted in Figure 4-2. The detailed integrated radiances are provided in Appendix Tables B-1 and B-2.

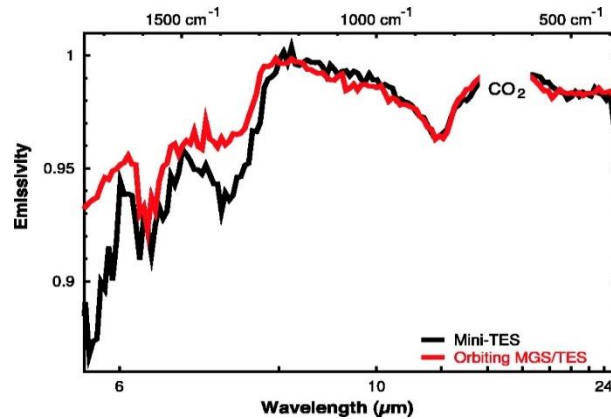


Discussion and Recommendations

Channel B (Figure 4-1) resulted in a larger polynomial fit as compared to Channel A. This was because of the large variation in the average pure mineral emissivity across this frequency band. The key advantage to the Channel A is that the range of emissivity at $25.2\ \mu m$ was $0.82 - 0.98$ with an average of 0.93 , while Channel B ranged from $0.47 - 0.90$ with an average of 0.63 . This difference in variability is demonstrated in the fit of the two series with the larger variability in the emissivity equating to a larger slope in the polynomial fit. This also translates to larger errors as shown in Figure 4-2. In the case of Channel A, the average error was static and about $6.6\% \pm 5.5\%$ for each temperature. Channel B increased from 7.3 to $8.5\% \pm 5.5\%$ with temperature. The standard deviation was static at about 5.5% in both channels. If an unknown pure mineral was encountered, the error could be as much as 9% in Channel A and 27% in Channel B.

The mineral spectral data sets used for this analysis relied on collected minerals. The emissivity error was calculated for each channel, but the question remains, what would the spectral error be for undisturbed, Mars bulk surface materials? A Mars bulk surface spectrum taken by Mini-TES (Figure 4-3)

Figure 4-3: Mars bulk surface spectra, Mini-TES, (Spirit, Sol 3, sequence P3004)



(Christensen et al., 2004) was downloaded and analysed with the methods of this section for Channels A and B (Spirit, Sol 3, sequence P3004). For this bulk spectrum, Channel A had an average emissivity of 0.987, resulting in an error of $1.12 \pm 0.12\%$. Channel B had an average emissivity of 0.929, resulting in an error of $3.19 \pm 0.77\%$.

This first order analysis demonstrates that the approach was valid, but that these forms of error must be considered in evaluation of the actual system performance (Section 6-4) and the total error budget (Table 6-9).

4.3 Reflectance model: basic

The objective of this analysis is to demonstrate that the integrated channel radiance calculation (Equation 4-1) matches the reflectance from mineral spectra. A non-hydrated mineral and a poly-hydrated mineral were selected as examples. The resulting concave features visually demonstrate hydration features.

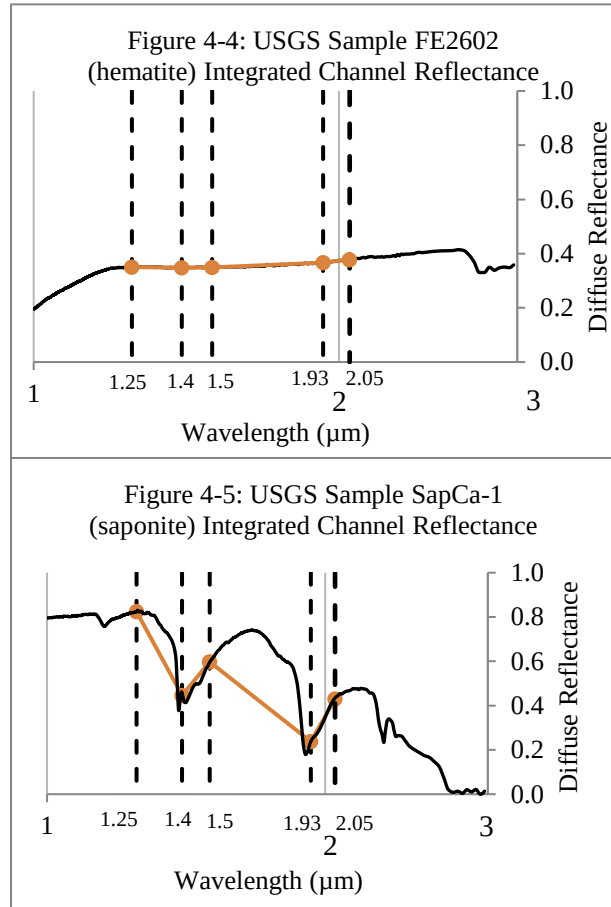
Methods

Spectral data for hematite (FE2602) and saponite (SapCa-1) were selected from the USGS database as examples of a non-hydrated and hydrated mineral, respectively (also see Section 2.6). Saponite has both bonded OH^- and H_2O . Integrated channel radiances were calculated from Equation 4-1. These channel radiances were connected with straight lines to

visually demonstrate the concave features associated with a hydration feature at 1.4 μm or bonded water at 1.93 μm , or the lack of these features.

Results

The result for the non-hydrated mineral, hematite, is provided in Figure 4-4. The result for the hydrated mineral, saponite, is provided in Figure 4-5. The channel radiances are plotted as orange circles.



Discussion and Recommendations

The hematite spectrum was flat with no absorption features at 1.4 or 1.93 μm . The saponite spectrum, as an example of a hydrated mineral with both OH^- and H_2O features, had pronounced absorption

features at both 1.4 and 1.93 μm . Lines connecting these five points demonstrated the concave features of the 1.25-1.4-1.5 μm combination and the 1.5-1.93-2.05 μm combination.

These results gave confidence that the underlying physical properties could be modelled, for at least single mineral substances. The next step was to determine the performance of the system with simulated spectra of mixed minerals with a linear mixing model.

4.4 Linear mixing model – preliminary reflectance calculations

A linear mixing model (as described in Section 1.8) was generated with mineral spectra measured in the University of Oxford Planetary Spectroscopy Facility. A non-hydrated mineral, weathered basalt, and a hydrated mineral, gypsum, were used for the measurements and models. Integrated channel reflectances were calculated and compared to the synthetic spectra. These

synthetic mixed spectra were then compared to measured physically mixed samples of basalt and gypsum.

Methods for the calculation and evaluation of linear mixing models

Two samples were prepared by the methods in section 2.3. These were the weathered basalt sample collected from Morocco and the gypsum sample from Pomaia, Italy.

Mixed sample preparation

Minerals were dry-sieve separated into 500-710 μm particle sizes. One gram total of each mixed samples were prepared by mass ratio distribution (Table 4-1). The mass ratios were converted into volume distributions for the linear mixed synthetic spectra calculations.

Table 4-1: Sample mixing ratios

Mass Ratio		Volume Ratio	
Basalt	Gypsum	Basalt	Gypsum
1.0	0.0	1.0	0.0
0.7	0.3	0.67	0.33
0.5	0.5	0.47	0.53
0.3	0.7	0.27	0.73
0.0	1.0	0.0	1.0

Spectra Measurement

Pure and mixed samples were measured with a Bruker IFS 66v spectrometer. The Bruker was setup with a Specac diffuse reflectance jig, calcium fluoride (CaF_2) beam splitter, a DTGS detector, and a quartz halogen source. The spectrometer measurement settings were: a spectral range from 4000-10000 cm^{-1} , aperture of 8 mm, gain of 4, and 250 scans. The mineral spectra were normalized to KBr powder as a spectrally flat reference.

Linearly mixed synthetic spectra calculations

Linear mixed synthetic spectra were calculated by adding volume-weighted ratios of each of the measured spectra for the pure samples of basalt and gypsum at each wave number. Ratios of these were calculated for each wave number by multiplying the pure mineral spectral reflectance value by the weighted ratio individually and then adding the result together.

Channel reflectance difference and ratio analysis compared to synthetic spectra

The combination of basalt (non-hydrated) and gypsum (hydrated) were analysed to understand the potential of linear mixing models for the interpretation of measured channel reflectance data. The methods were band difference analysis (one reflectance band subtracted from another) and band ratio analysis (one or more bands divided by another).

Channel Difference Analysis

A band difference comparison of two sets of two channels was run: a) 1.5 μm subtracted from 1.4 μm , and b) 1.93 μm subtracted from 1.25 μm . Synthetic values were calculated from 0 to 100 percent gypsum in the sample at 5% intervals (plus 1% and 99%).

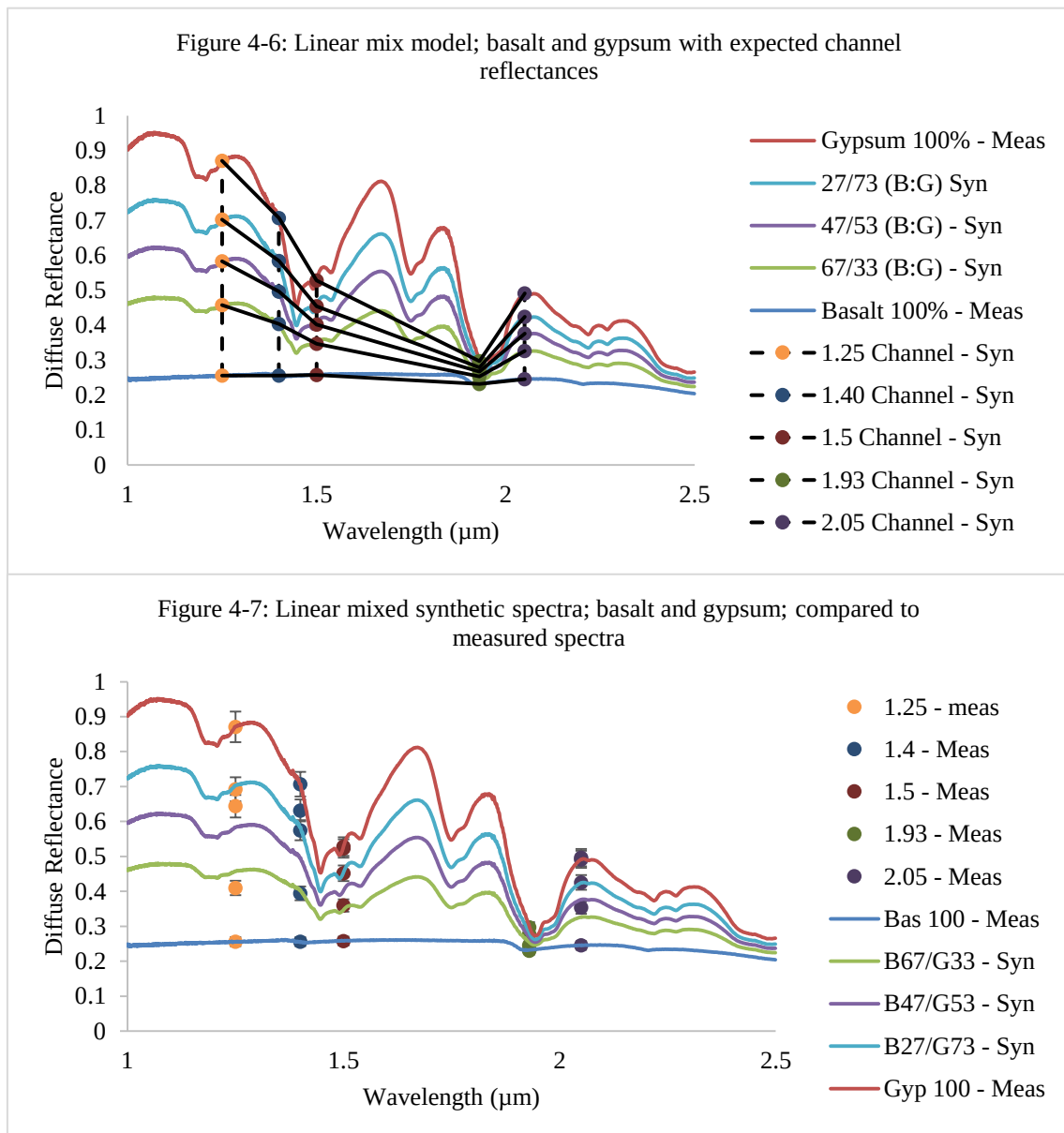
Channel Ratio Analysis

A band-depth ratio was run for several 2 channel and 3 channel configurations: a) 1.4/1.5, b) 1.25/1.93, c) (1.5+2.05)/1.93, d) (1.25+2.05)/1.93, and e) (1.25+1.5)/1.4.

Results

Linearly mixed synthetic spectra calculations

The linearly mixed synthetic spectra are plotted in Figure 4-6.

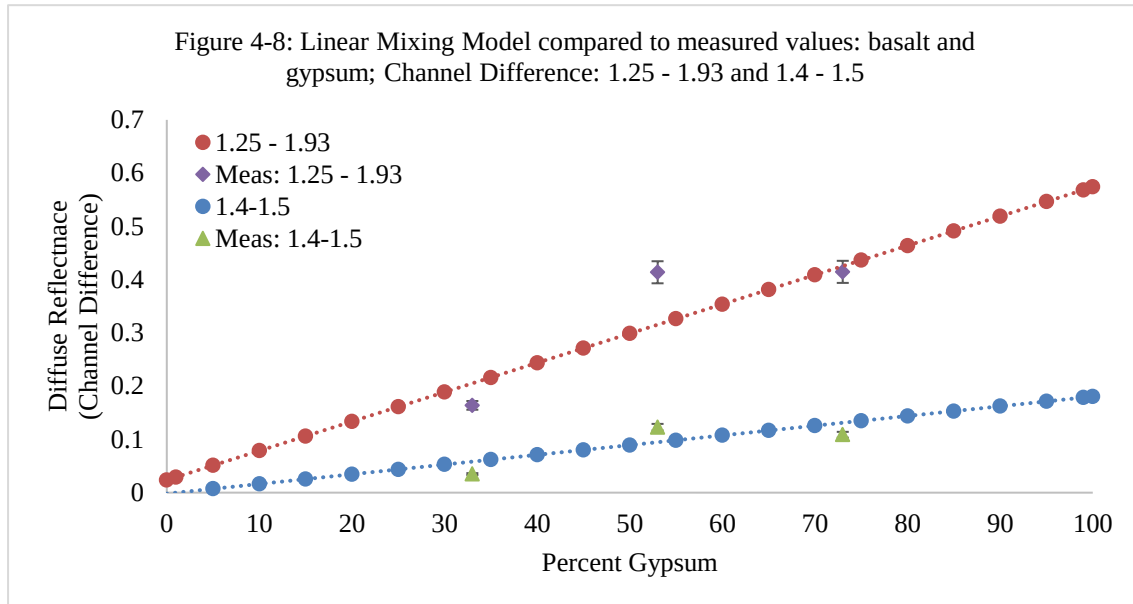


Comparison of synthetic spectra to measured channel radiances

The linear mixed synthetic spectra were compared to the measured data in Figure 4-7.

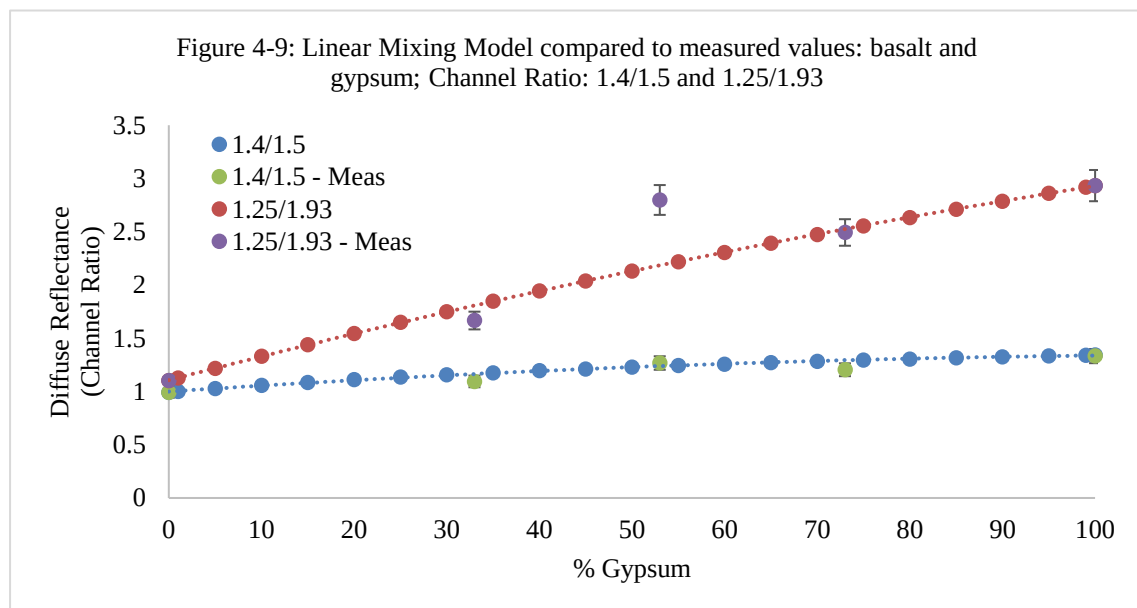
Channel Difference Analysis

The two sets of two channels difference analysis results are plotted in Figure 4-8.



Channel Ratio Analysis

Figure 4-9 presents the 2-channel ratios. The measured data indicates that the error is $\pm 40\text{-}50\%$. Figures 4-10, 4-11, and 4-12 present 3-channel ratios.



Discussion and Recommendations

Linearly mixed synthetic spectra calculations

The expected channel reflectances are graphed as single points on the graph in the 5 channels (Figures 4-6). These are connected by straight lines because, in the integrated instrument, it is possible to use the shape of the connected points in addition to the band ratios to discriminate minerals and mineral mixtures has been done on ExoMars with Pancam ((Cousins et al., 2010).

Comparison of synthetic spectra to measured channel radiances

As can be seen in Figure 4-7, the variability between the measured data and synthetic data was significant with errors in the measured data of $\pm 5\%$ relative

reflectance. This is noted as the integrated reflectance (circles) not aligned with the synthetic spectra positions. Still, while the intensities may not be correct, the measured data follows the form of the synthetic data with absorption features in the correct location. The issue remains if this is good enough for determination of the hydration features (e.g., positive or negative detection) and/or if it will be enough to determine the percent concentration of the minerals.

Figure 4-10: Linear Mixing Model; basalt and gypsum; Channel Ratio: $(1.5+2.05)/1.93$

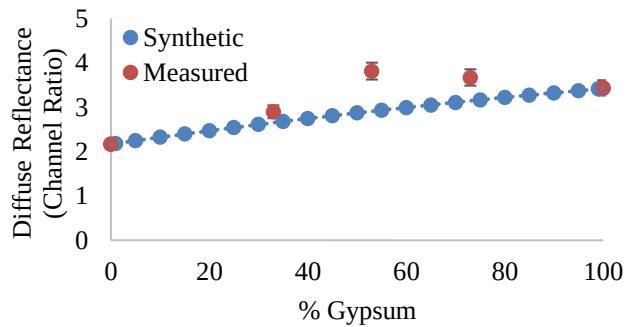


Figure 4-11: Linear Mixing Model; basalt and gypsum; Channel Ratio: $(1.25+2.05)/1.93$

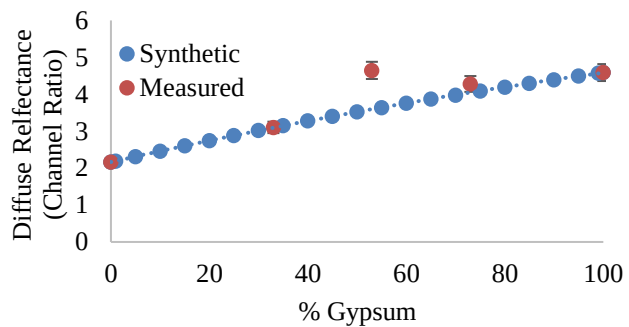
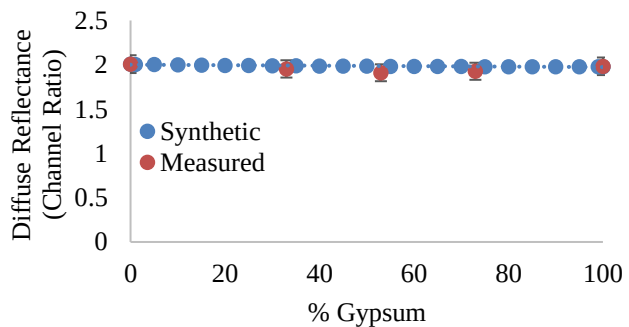


Figure 4-12: Linear Mixing Model; basalt and gypsum; Channel Ratio: $(1.25+1.5)/1.4$



Channel Difference Analysis

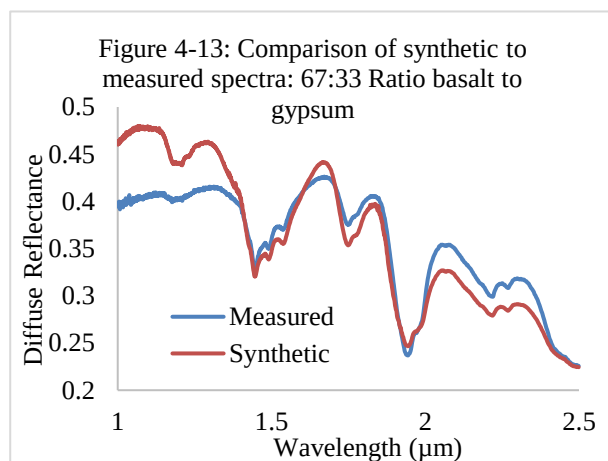
The measured data were significantly beyond the linear fit of the synthetic channel difference data in Figure 4-8. There is at least a $\pm 25\%$ error in both the 1.4 - 1.5 μm and 1.25-1.93 μm channel difference. The dynamic range of the 1.4-1.5 μm difference is about 0.18 while the dynamic range of the 1.25-1.93 μm difference is about 0.57.

Channel Ratio Analysis

Like the difference analysis, synthetic values were calculated from 0 to 100 percent gypsum in the sample at 5% intervals (plus 1% and 99%) (Figure 4-9). The measured data in the same ratios are plotted for each configuration. The errors range from $>50\%$ to 100% in the case of Figure 4-12. The ranges for the channel ratios were 1.27, 2.43, and 0.11, respectively for Figures 4-10, 4-11, and 4-12. The $(1.25+1.5)/1.4$ μm ratio was effectively flat. This was reasonable because gypsum does not have an OH^- absorption feature at 1.4 μm .

General

The measured sample spectra can have results that align well with the synthetic linear mixed spectra as is shown in Figure 4-13. Both the shape and the intensity is well matched throughout the spectra; however, there are multiple variables that affect the spectral response that can cause errors where the measured spectra match the general shape, but not the intensity. This can cause large errors if a precise measurement of percent concentrations of the minerals is necessary as is shown in Figure 4-7 where the measured channel radiance have significant error and differences compared to the synthetic spectra.



Another potential issue is the dynamic range. The instrument will have to have suitable sensitivity in order to discriminate mineral abundances. As an example of the importance of good dynamic range, Figure 4-12, shows that a flat mineral spectra would render this ratio unusable for the determination of the ratio of gypsum to basalt. Choosing ratios with a good dynamic range

will help the overall performance of the instrument; however, a specific requirement was not specified in Table 3-8.

Finally, linear mixing models provide limited results because natural samples are more typically unevenly distributed intimate mixtures rather than separated discrete minerals. The determination of mineral abundances is difficult because the spectra are in reality complex nonlinear functions of grain size, abundance, and material opacity (Hapke, 2012, Poulet et al., 2002, Shkuratov et al., 2012). It is necessary to consider a non-linear mixing model. This is discussed in the next section.

4.5 Hapke Model – Overview, Emery Widget, Optical Constant Fitting

It was shown in the previous section that linear mixing models deviate from the measured data by around $\pm 5\%$ with error in the channel difference and ratio analysis of around $\pm 25\%$. This is because spectra are complex nonlinear functions of grain size, abundance, material opacity, and multiple reflection.

Measuring the Bidirectional Reflectance Distribution Function (BRDF) is a common method for remote sensing of planetary surfaces in order to map surface mineral composition (Hapke, 2012). The BRDF is defined as, *the ratio of the radiance scattered from the surface of a medium into a given direction to the collimated power incident on a unit area of the surface* (Hapke, 2012). The reflection of light off of a surface depends on i) viewing angle, ii) direction of the light source, iii) shape of the material particles, iv) topology of the surface, v) compositions of the material, and vi) packing arrangements (Helfenstein and Shepard, 2011, Wong et al., 2014).

Other materials could absorb reflected radiation in a way that masks the principle water or hydrated mineral bands at 1.4 μm and 1.93 μm . It is important to select predominate materials, such as pyroxenes (e.g., augite), on the surface of Mars that have features in these bands and mix these with water and/or hydrated mineral spectra to determine if they will mask the 1.4 μm hydroxide and 1.93 μm water ice features.

The most typical approach to non-linear mixing models are the methods developed by Hapke (1981, 1984, 1986, 1993). This approach calculates an approximate solution to the

radiative transfer equation that describes the emission, absorption, and scattering of light on a non-uniform particulate surface (DeMeo, 2010, Emery, 2002, Poulet et al., 2002, Shkuratov et al., 2012). These methods are utilized for all non-linear mixing models as part of this thesis.

In this section, the methods of calculating Hapke models are presented, the Emery IDL widget for running the calculations is introduced, and optical constants that were obtained for this analysis were matched to measured mineral spectra using the Emery widget.

Hapke Model Description and Equations

The Hapke model is used to determine the bidirectional reflectance distribution function (BRDF), most of which have low single-

scattering albedos and are not highly anisotropic.

The original form (Hapke, 1981) calculates the total radiance from the sum of single-scattering and multiple-scattering radiances (Liang and Townshend, 1996). Depending on the version of the model, 6 parameters are required which link multiple scattering, the phase function, the

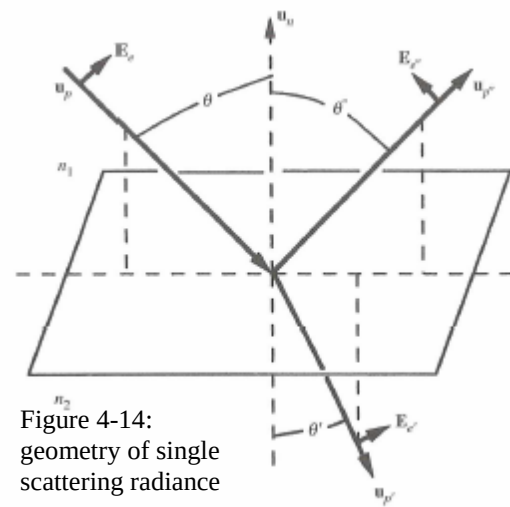


Figure 4-14:
geometry of single
scattering radiance

opposition effect, and surface roughness (Cord et al., 2003). The incident light is separated into two components: a collimated component which has penetrated in-between the particles and a diffuse light that has been scattered multiple times (Emery, 2002). The single scattered radiance is calculated by integrating over the volume penetrated, while the multiple scattered radiance is calculated by a two-stream approximation for isotropic scattering in which the light is divided into an upward-going hemisphere and a downward-going hemisphere (Figure 4.14).

Approximations and Assumptions

There are a number of approximations that serve to reduce the complexity of the Hapke model, as well as limit the applications.

- Most soils have low single-scattering albedos and are not highly anisotropic. This is important because angular patterns cannot be predicted when soil scattering is very strong and anisotropic (Liang and Townshend, 1996).

- Retrieved particle single-scattering albedo depends on the compaction state of the samples (Helfenstein and Shepard, 2011, Shepard and Helfenstein, 2011, Shkuratov et al., 2012).
- Diffuse reflected light is considered; any specular component is ignored (Wong et al., 2014).
- The larger number of parameters (9-10) allows a fit that may not be unique or representative because too many degrees of freedom allow a fit to just about anything. This also significantly increases processing time (Cord et al., 2003, Liang and Townshend, 1996, Schmidt and Fernando, 2015, Shkuratov et al., 2012, Souchon et al., 2011).
- Specific assumptions from the Hapke 1981 model (Walker, 1998):
 - Collimated source
 - Sample contains randomly oriented, partially absorbing particles of irregular shape.
 - The particles are large compared to the wavelength of the light.
 - The scattering particles are imbedded in a medium of refractive index of $n = 1.0$.
 - Light is absorbed according to Beer's law.
 - A two stream solution may be used for the multiple scattering component.
 - A first-order approximation to the non-isotropic multiple scatter result is obtained by using the multiple scatter result for isotropic scatterers because the multiple scatter term is less sensitive to the single particle scattering phase function.

Theory

The model spectra are generated per Equation 4-2 (taken from equation 16 of Hapke (1981)). These were used as the basis for the development of an IDL widget by Josh Emery that generates a Hapke derived mixed spectra.

$$r(\mu_0, \mu, g) = \frac{w}{4\pi} \frac{\mu_0}{\mu_0 + \mu} \{ [1 + B(g)]p(g) + H(\mu_0)H(\mu) - 1 \} K \quad \text{Equation 4-2}$$

Where:

Parameter	Description	Parameter	Description
$r(\mu_0, \mu, g)$	Bidirectional reflectance	w	Single scattering albedo (Equation 4-3)
μ_0	Cosine of angle of incidence	$B(g)$	Backscattering function
μ	Cosine of angle of emergence	$p(g)$	Surface phase function
g	Phase angle	$H(\mu_0)H(\mu)$	Multiple scattering function
K	porosity		

$$w = \frac{\sum_i \frac{m_i}{\rho_i d_i} Q_{Si}}{\sum_i \frac{m_i}{\rho_i d_i}} \quad \text{Equation 4-3}$$

Where w is calculated as the weighted average of the scattering efficiency (Q_{Si}) of each particle in a multi-component surface, m_i is the mixing ratio, ρ_i is the solid density, d_i is the particle diameter, and Q_{Si} includes both the real and imaginary indices of refraction of the material.

An important step is to confirm the validity of the Hapke model by comparison to measured physically mixed samples; however, the Hapke model is dependent upon having optical constants from the minerals under study. These are difficult to measure and few exist (Roush, 2005, Roush et al., 2007). Therefore, a subset of configurations were selected that allow demonstration of the validity of the Hapke models to identify the hydrated mineral features and the potential for mineral discrimination. These were further limited to those having both the physical sample and appropriate optical constants (Table 2-5).

The development of methods for physically testing water ice/mineral mixtures formed in a Mars type process was beyond the scope of this thesis. These non-linear mixing models, combined with integrated system models in Chapter 5, form the majority of the analysis of the capability to be able to detect water ice with simulated spectra.

Emery IDL Hapke Mixing Model Widget Description

A computerized model developed in IDL was utilized for the Hapke modelling. An IDL widget was developed by Emery (2002) as part of doctoral thesis work to calculate non-linear Hapke models applied to airless bodies, asteroids in particular. Calculations are described in two other papers published post thesis work (Emery and Brown, 2004, Emery et al., 2006). This model is based on 1993 updates to the Hapke model (Hapke, 1993, 2012). This section provides background information necessary to understand how the mixed spectra were calculated for this thesis and the limitations of the results, but is not meant to be an exhaustive review.

Assumptions and Limitations of the Emery Widget

There are a number of important assumptions in this code. While based on the standard Hapke assumptions and limitations, they are repeated here for clarity (Emery, 2002):

- The particle diameter is at least 3-4 times larger than the wavelength.
- Emery ignored the effects of surface roughness because of uncertainties about the physical state of surface materials on airless bodies. This is also the assumption for borehole surfaces.
- Assumes isotropic scattering.
- Assumes that the surface is composed of a mixture of grains that are each of a single composition. This is a “salt and pepper” mixture. In this case, the

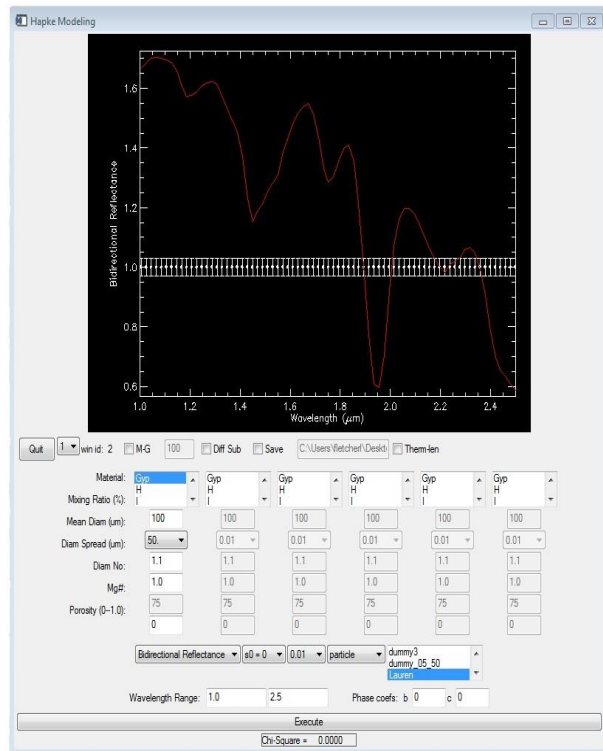


Figure 4-15: Emery IDL widget user interface.

- photon will only encounter one type of composition at a time, but may be reflected multiple times from multiple types of composition.
- A 1- σ error of 3% was assumed in the model. For the purposes of this thesis, all errors associated with the Hapke Model will be 3- σ , or $\pm 10\%$. These are not graphed for clarity.

Functions of the Emery Widget

The widget has a number of input parameters as can be seen in Figure 4-15 with an example of pure gypsum with a particle diameter size of 50 μm . The key parameters utilized in this thesis included the materials, mix ratios, particle diameters, and frequency range with the rest ignored. Up to six minerals could be evaluated in a single mixture as long as the total combined percentage was 100. Particle diameter sizes can be varied from 0.01 μm to a size that produces lambertian scattering; however, the smallest particle size allowed by the Hapke model limitation is 3-4 times the wavelength.

The widget required the optical constants, both real and imaginary components, through the measured frequency range (1-2.5 μm), and the density for each material evaluated.

Material selection, source of optical constants and material density data, and mixture ratios

The materials selected for the Hapke model were from those that were identified as materials on the surface of Mars (Tables 1-3 and 2-2), that could be obtained (Table 2-4), and for which optical constants existed (Table 2-5).

The mix ratios for water ice mixtures will be for Hapke modelling while the mineral mixtures will be physically tested in the spectrometer per the methods of section 4.4 and compared to the Hapke models. These mixtures are provided in Table 2-7.

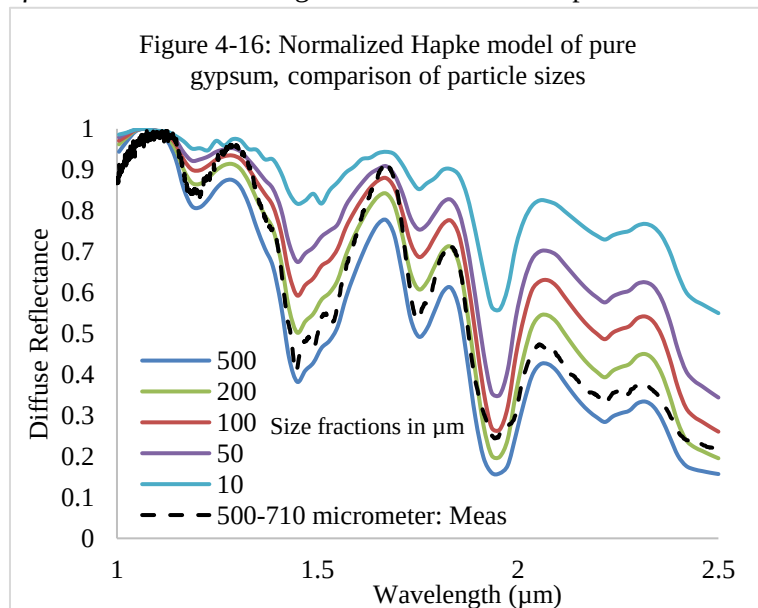
Fitting Hapke models of pure un-mixed minerals to measured spectra

The particle size fraction of the mineral is one of the key parameters that affects the shape of the calculated spectra. As the particle size gets smaller, the shape of the spectra flattens out and spectral features are lost. The gypsum, basalt, and JSC Mars-1 minerals were dry-sieve separated into a size fraction of 500-710 μm ; however, there were fine particles that clung to the larger particle surfaces. These can change the spectral shape by adding multiple reflections. While the Hapke widget can be programmed with a variety of particle sizes, the first step is to match the Hapke model output to the measured spectra to ensure that the base properties are correct.

Method

The Hapke widget was programmed to analyse a pure mineral across a number of particle sizes (in μm) as follows: 10, 50, 100, 200, and 500. The lower particle size limit was set to 10 μm to be 4 times larger than the 2.5 μm maximum wavelength evaluated in the Hapke model, as is required in the assumption.

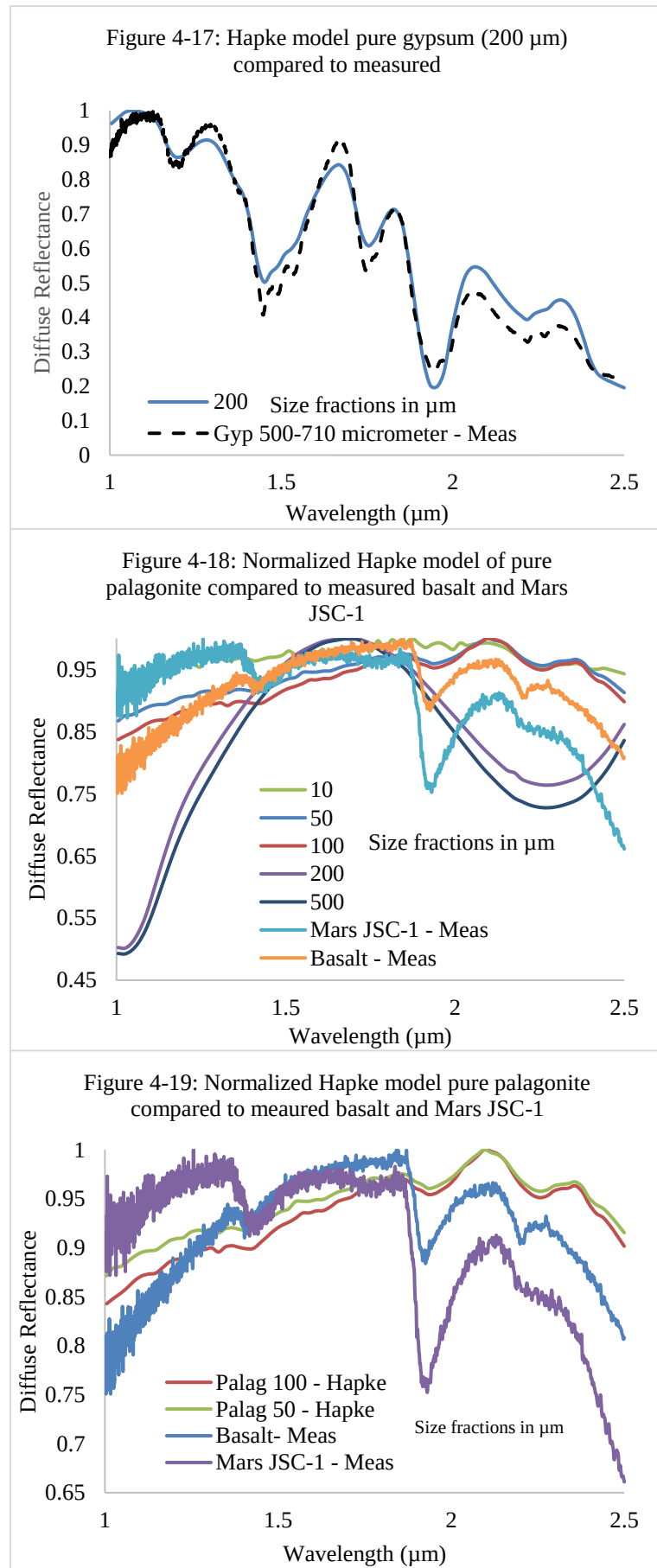
These were plotted against the measured spectra in order to determine a best fit. Hapke calculated and measured data were normalized to the maximum value set to 1 by dividing all the values in the series by the maximum series



value. This method was applied to all samples individually to allow them to be compared. The band positions and relative band-depths were maintained with this approach. Hapke generated spectra were fit to measured spectra for gypsum, basalt, Mars JSC-1, pyroxene, and water ice. The spectral range is plotted against the Hapke model generated spectra or diffuse reflectance for the measured spectra.

Results

The Hapke spectra for gypsum are plotted in Figure 4-16. The final fitting for the gypsum Hapke model to the measured result is shown in Figure 4-17. The Hapke spectra were generated for a Palagonite and are plotted against measured data for basalt and Mars JSC-1 in Figure 4-18 with the final fitting in Figure 4-19. The Hapke spectra for pyroxene are plotted in Figure 4-20.



The Hapke spectra for water ice are plotted in Figure 4-21. These are plotted against two measured spectra for water ice: 1) GSD136 at 77 K temperature (Clark et al., 2007, downloaded from USGS Spectral Database), and 2) Water ice measured at 236 K (Clark et al., 1986). The final fitting for the water ice spectra at 236 K are plotted against 500 μm particle size in Figure 4-20.

Discussion/recommendations

Generally, all of the Hapke modelled spectra matched the measured data in terms of shape. As previously noted, there are fine particles that cling to the larger particle surfaces. These have the effect of changing the spectral shape and intensity by providing additional reflection pathways for the incident radiation. The best fit for the available model configurations are described in the following paragraphs.

Figure 4-20: Hapke model pure pyroxene, comparison of particle sizes

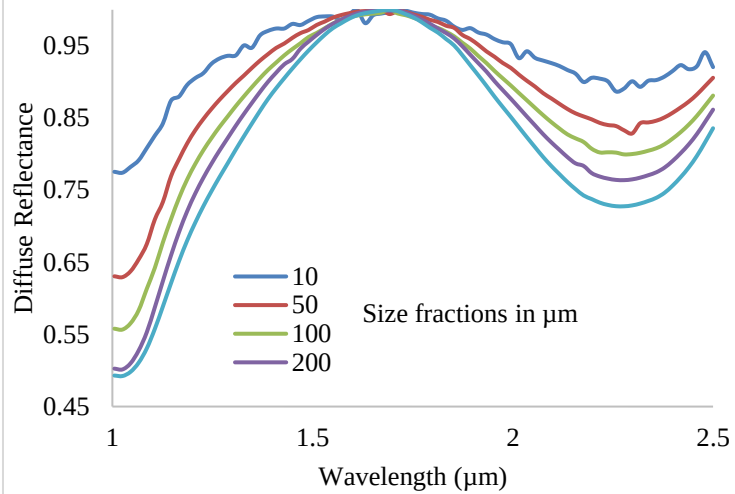


Figure 4-21: Normalized Hapke model of water ice compared to measured values

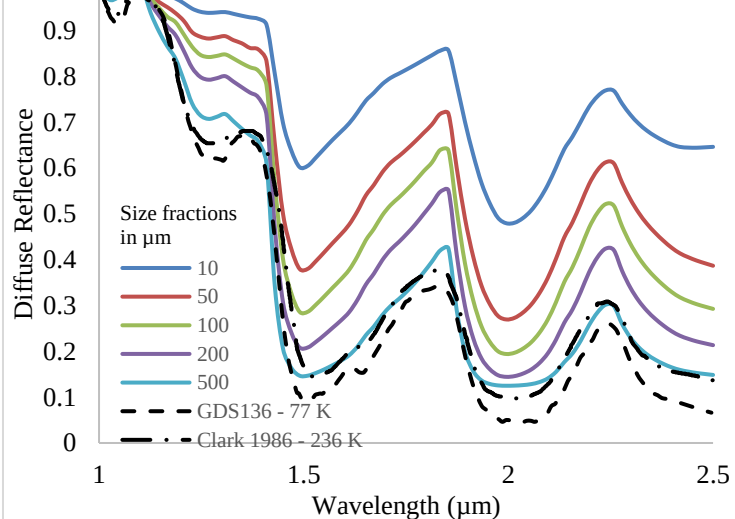
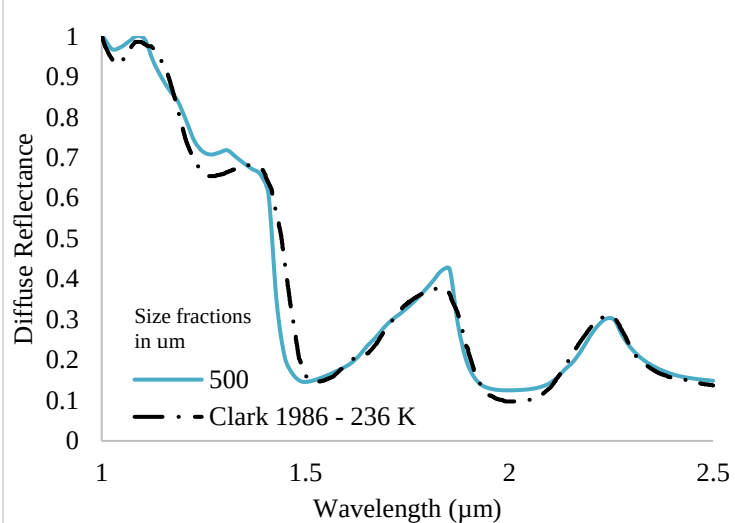


Figure 4-22: Hapke model water ice compared to measured ice



Gypsum

The best fit for gypsum was the 200 μm particle size distribution, which would suggest that the dry-sieving method was insufficient to separate the finer particles from the larger particles. Washing is an additional step that could be used to separate the small from the large particles; however, gypsum is slightly soluble so washing this is not a viable option without altering the mineral composition. As a result, the 200 μm size fraction for gypsum will be used for the mixed mineral Hapke models.

Basalt and Mars JSC-1

Basalt and Mars JSC-1 measured data resulted in nearly identical curves (Figures 4-18 and 4-19). For the Hapke model generated spectra, the larger particle sizes (200 and 500 μm) show an absorption feature at 2.3 μm that is typical of a pure pyroxene (e.g., pigeonite and augite), while the rest demonstrate features more typical to a weathered sample. Weathering effects include reducing the spectral contrast (flattens the shape) and the addition of water features by water absorbed to the surface. The best fits, while not ideal, were the 50 μm and 100 μm curves (Figure 4-19) which follow the shape of the measured basalt and Mars JSC-1. The 100 μm palagonite curve will be used for a Hapke model with water ice to serve for both basalt and Mars JSC-1

Pyroxene

The pyroxene spectra have a distinct “S”-shape with two important spectral features in the 1-2 μm range (Figure 4-20). The first is at about 1.05 μm and the second is at about 2.3 μm which are due to ferrous Fe located in the M2 crystallographic site (Schade and Wasch, 1999). These might affect the absorption features of a hydrated mineral at 1.93 μm and the anchor band at 1.25 μm when mixed with hydrated minerals, masking the signal. Therefore, the spectra for 500 μm particle size will be used as the worst-case configuration in the mixed models with water ice as it had the largest depth of the absorption features.

Water Ice

The water ice spectra in Figure 4-21 show that the spectra at 236 K, which is within the temperature range on Mars, provides the best match to the Hapke model for 500 μm particle size

(Figure 4-22); therefore, the spectra for the 500 μm particle size will be used in the mixed models with water ice.

4.6 Water Ice Mixture Hapke Models

The Hapke generated spectra for water ice were mixed with palagonite to simulate the Morocco basalt and JSC Mars-1 samples and then with pyroxene as a general non-hydrated mineral found on the surface of Mars. This section outlines the process for creating the Hapke generated mixed spectra, difference and ratio analyses applied to the data, methods for evaluation of valid relationships between the channels, identifies limits to the method for the detection and discrimination of water ice in a non-hydrated mineral matrix, and makes recommendations for a future integrated instrument.

Methods

The particle sizes were set to 500 μm for water ice, 100 μm for palagonite, and 500 μm for pyroxene (see Section 4.5). Sampling was set from 1 to 2.5 μm frequency range. Density and optical constants were used as specified in Table 2-5. Percentage mixtures were run per Table 2-7. Integrated channel radiances were calculated from the mixed spectra.

These channel values were then used as part of a channel difference and ratio analysis to determine which of the channel relationships could be used in the detection and quantification of water ice (Table 4-2).

Table 4-2: List of channel difference and ratio analyses

	Formula	Comment
1	$1.25 - 1.5$	Two-point difference around 1.4 μm water absorption band
2	$1.4 - 1.5$	Two-point difference to 1.4 μm hydroxide absorption band
3	$1.25/1.5$	Two-point Ratio around 1.25 μm water reflectance band
4	$1.4/1.5$	Two-point Ratio to 1.4 μm hydroxide absorption band
5	$(1.25+1.5)/1.4$	Three-point ratio to 1.4 μm hydroxide absorption band
6	$(1.5+2.05)/1.93$	Three-point ratio to 1.93 μm water absorption band with 1.5 μm anchor
7	$(1.25+2.05)/1.93$	Three-point ratio to 1.93 μm water band with 1.25 μm water reflectance band
8	$1.25 - 1.93$	Two-point difference around 1.93 μm water absorption band
9	$1.4 - 1.93$	Two-point difference around 1.93 μm water absorption band

In the evaluation of the performance of the channel analyses, there are three important criteria:

- 1) The values in the range of interest should be non-degenerate (e.g., no overlapping). While the science requirements (Table 1-4) call for discrimination of up to 15% water by weight, the best-case scenario would be to be able to detect and discriminate water from 0% up to 100%. A good result, noted with a “✓”, will mean there are no duplicate points in the full range (up to 15%), “-” will mean no duplicates in the minimum range, and “✗” will mean that there are duplicates in the minimum range.
- 2) There should be a good fit to the data in terms of a linear or polynomial fit; however, if it is a polynomial, it should be limited to a 3rd order because too many degrees of freedom would allow a fit to just about any dataset. This will indicate a reproducible trend with no discontinuities. This fit is necessary to convert the Hapke model calculated diffuse reflectance (denoted as ‘Hapke’ in the figures) to percent water. A good result noted with a “✓” will mean a fit with an $R^2 > 0.9950$, “-” will mean a marginal fit with an R^2 from 0.9900 to 0.9950, and “✗” will mean a poor fit with an $R^2 < 0.9900$. Adjusted R^2 values (noted as R^2_a in the figures) were calculated by $1 - ((1 - R^2) * (N - 1) / (N - p - 1))$ where N is the number of mixtures in the analysis (15 in all analyses) and p is the number of variables (11 from Equations 4-2 and 4-3).
- 3) There should be good dynamic range in the fit. This is important for the instrument because if the dynamic range is smaller than the instrument sensitivity, it will not be able to discriminate percent water. A good result noted with a “✓” will mean a dynamic range > 0.25 diffuse reflectance, “-” will mean a dynamic range from 0.1 to 0.25 diffuse reflectance, and “✗” will mean a dynamic range < 0.1 diffuse reflectance.

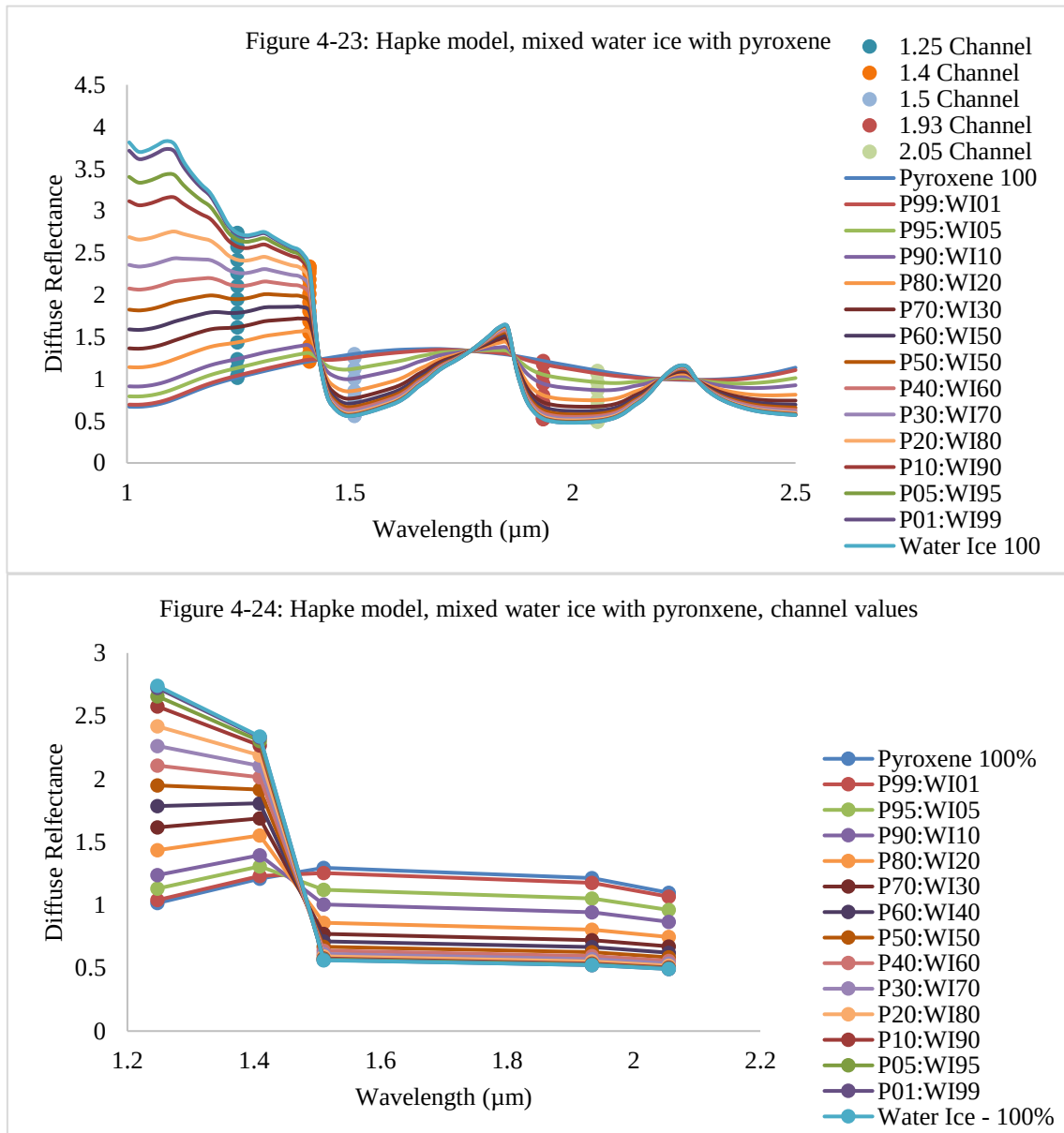
The steps for this analysis are as follows. 1) The Hapke calculated spectra for each mixture and concentration were plotted with the integrated channel radiances. 2) The spectral data were stripped away leaving just the integrated radiances. 3) These were normalized to a maximum value of 1 by dividing each of the integrated radiances by the maximum radiance of all values. 4)

Ratios and differences were calculated for the relationships established in Table 4-6. 5) These were analysed to determine if the results were valid under the criteria of: a) each data point in the resulting series was unique, b) a good fit, and c) good dynamic range.

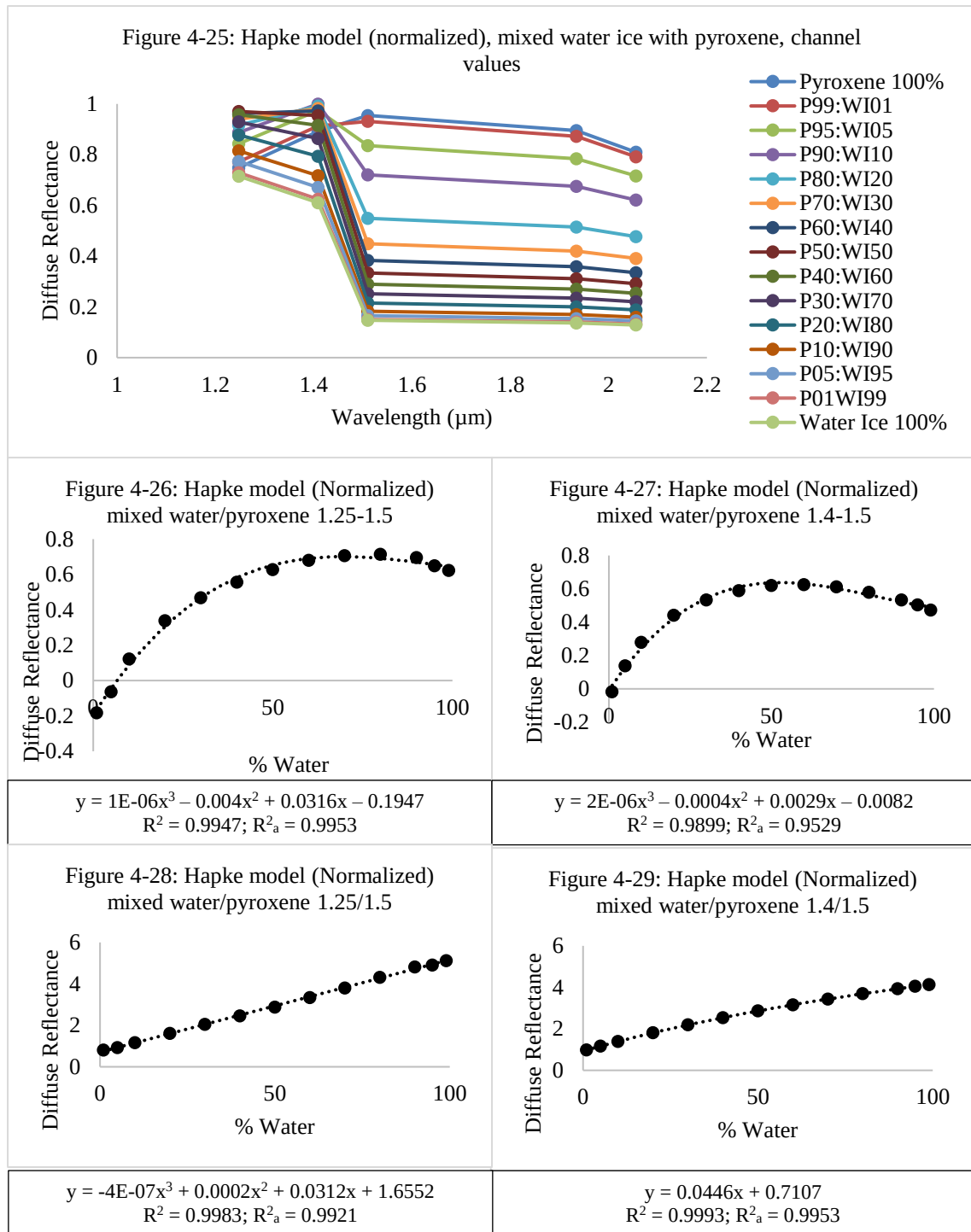
All the figures produced for pyroxene were reproduced for palagonite, though only those relevant are presented.

Results

Figure 4-23 shows the results of the Hapke model output by wavelength for each of the mixtures. Figure 4-24 shows a reduced version of the channel reflectances connected with straight lines for each of the water ice concentrations. Figure 4-25 shows the results for the normalized channel values. Figures 4-23 to 4-34 present the results for water ice mixed with pyroxene.



Figures 4-35 and 4-36 present the results for water ice mixed with palagonite. A summary of the



Discussion

Water Ice & Pyroxene

Figure 4-23 shows the results of the Hapke model output by wavelength for each of the mixtures. The values at the band-passes of 1.25, 1.4, 1.5, 1.93, and 2.05 μm are plotted on each of the spectra with solid circles representing the expected reflectance in that channel. The

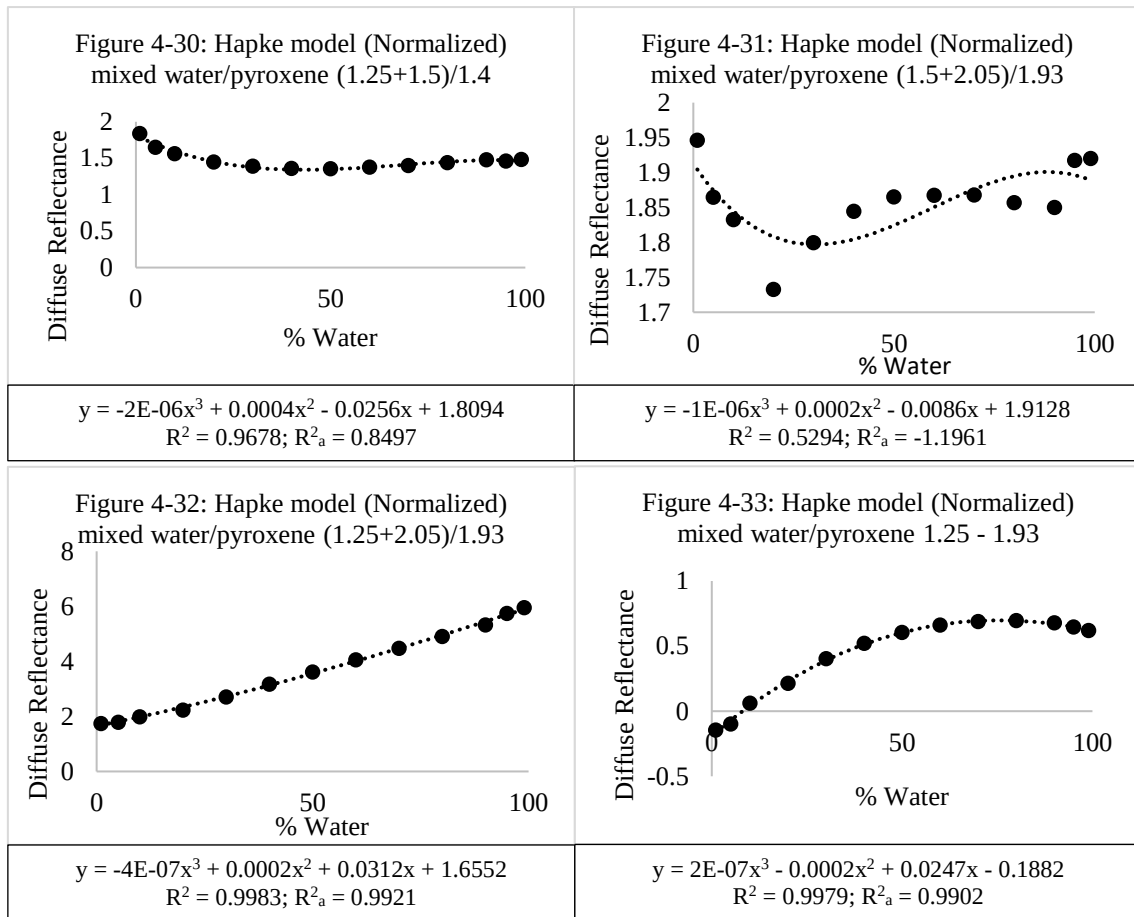
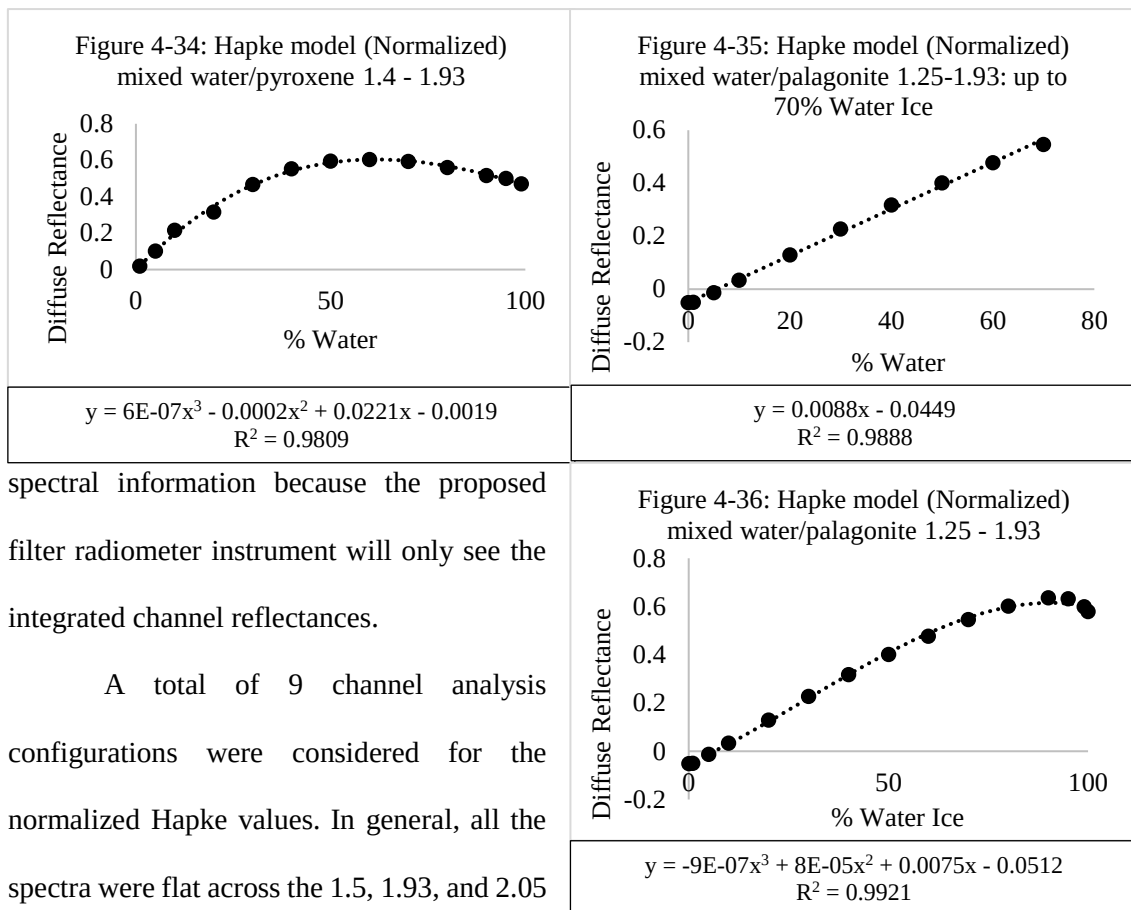


Table 4-3: Channel analysis performance for water ice with pyroxene and palagonite

	Analysis Channel Combination	Pyroxene			Palagonite		
		1 non-degenerate	2 Good Trend	3 Dynamic Range	1 non-degenerate	2 Good Trend	3 Dynamic Range
Normalized to max series peak value	1.25 – 1.5	✗	-	✓	-	✓	✓
	1.4 – 1.5	✗	✗	✓	✓	✓	✓
	1.25/1.5	✓	✓	✓	-	✓	✓
	1.4/1.5	✓	✓	✓	-	✓	✓
	(1.25+1.5)/1.4	✗	✗	✓	-	✓	✓
	1.25 – 1.93	-	✓	✓	-	✓	✓
	1.4 – 1.93	-	✓	✓	-	✓	✓
	(1.5+2.05)/1.93	✗	✗	✓	✗	✓	✗
	(1.25+2.05)/1.93	✓	✓	✓	✗	✓	✓

pure pyroxene sample is a fairly flat S-shape from 1 to 2.5 μm around the Hapke model calculated reflectance = ~ 1 . Water has a dramatic affect to these spectra with strong absorption features at 1.5 and 2.0 μm and increasing reflectance below 1.4 μm . All 5 bands have variation that appear to be directly connected to the increasing water ice content. The next step was to strip away the



The three analyses that satisfied all three criteria for the normalized data sets were the 1.25/1.5, 1.4/1.5, and (1.25+2.05)/1.93 μm ratios. The rest were either completely eliminated or are only good in the minimum range (1-15%). These are compared to the results of the analysis of mixed water with Palagonite to determine if there is a universal analysis combination that can be used independently of other surface data sets or if additional information will be required.

Water Ice with Palagonite

The results were visually similar to the pyroxene with flat spectra across the 1.5, 1.93 and 2.05 μm bands, as was expected for water ice mixtures (Figures not presented); however, the channel analyses were significantly different (Table 4-3). In particular, the 1.93 μm three channel combinations were eliminated. The only analysis that satisfied all three criteria was the 1.25-1.93 μm difference (Figure 4-35); however it is limited in the upper range, so is only good for up to

~70% water ice content (Figure 4-36). The rest were either completely eliminated or are only good in a much more restricted percent water ice range.

Water Ice Hapke Model Summary

Spectra from the Hapke models of water ice with two typical Mars spectral analogues were flat from across the 1.5, 1.93, to 2.05 absorption bands. It was expected to generate an L-shape from the reduced channel values across the five channels in spectrometer mode (e.g., assessing all five channels simultaneously) (Figure 4-25). The five channels were originally selected to also account for hydrated minerals in addition to water ice; however, the selection of the 1.25 μm as an anchor band for hydrated minerals turned out to be the most useful correlation to the presence and quantification of water ice when mixed with pyroxene and palagonite. This is because the water ice becomes more reflective at higher concentration in this region of the spectrum and significantly increased the dynamic response range when assessed with the 1.93 μm band. Because pyroxene has a strong 2 μm absorption band, it wasn't clear how that would affect the water ice absorption feature at 1.93 μm , but in the end it appears to have no effect on the usefulness of the 1.93 μm absorption feature in connection to the 1.4, 1.5 or 2.05 μm bands as these are flat across all concentration mixtures (Figures 4-23 and 4-24). From visual inspection of Figure 4-23, it would appear that anchor bands at 1.85 μm and 2.25 μm would help to bring out the 1.93 μm feature when assessed for water ice; however, since these bands are also specified to accommodate hydrated minerals, this must be considered after an analysis of the Hapke models of mixed minerals.

The best channel combination for both pyroxene and palagonite was the 1.25-1.93 μm difference. It had the best fit and good dynamic response range, though it is limited to ~70% water ice content before it degrades. Since this meets the science requirements of detection and discrimination of 1 to 15% (Table 1-4), this is an acceptable limitation and is recommended as the principal channel for the detection and discrimination of water ice.

When comparing channels from pyroxene to palagonite, the general scale is closely matched. The shape is the problem, where the palagonite has a lower overall reflectance that is most likely due to a higher emissivity than the pyroxene.

Because the capability to discriminate the water ice percentage is most directly affected by the instrument sensitivity, the dynamic range performance must be confirmed with integrated instrument calculations and testing with these Hapke spectra. This will be presented in Chapters 5 and 6.

Another key issue on quantification of water ice is that it is very probable that, depending on the material, different ratios will be necessary for different concentrations, especially in the high water ice concentration mixtures. For palgonite, Fig 4- 35, the 1.25 – 1.5 difference can be used for <70%, but would have to be switched to the 1.4/1.5 ratio channel for percent concentrations >70%. Having multiple channels is quite useful for correlation of water ice concentrations.

The best case would be that one band could be used to determine water percentage independent of knowledge of the material prior to subsurface measurement. This would appear to be difficult and that additional information from surface work is necessary to provide a starting context to bound the results. Additional data types that could aid this are discussed in Section 5.8.

4.7 Hydrated Mineral Detection Hapke Models

One of the primary science objectives is for the detection of hydrated minerals (Table 1-4). This will be a positive or negative detection, only. The next section (4.8) will address the potential for discrimination of mineral mixture percentages. For this requirement, it was proposed to utilize the 1.4 μm and 1.93 μm absorption features that indicate bonded OH^- and H_2O , respectively. A key limitation in this analysis was the availability of optical constants for the minerals identified as being present on the surface of Mars. These were necessary for the Hapke models. A small number were obtained for gypsum, serpentine, illite, kaolinite, saponite, and montmorillonite. These were mixed with pyroxene and palagonite.

Methods

The minerals were mixed with methods similar to the water ice models (see Section 4.6). Mineral spectra were obtained from the USGS spectral database and were fit to a particle size generated by the Emery Hapke widget for a pure mineral following the methods from Section 4.5 (data not provided, but refer to Figure 4-16 as an example). A listing of the hydrated minerals, sources, and particle size fit for the Hapke model are provided in Table 4-4.

Table 4-4: Hydrated Mineral details for Hapke model generation

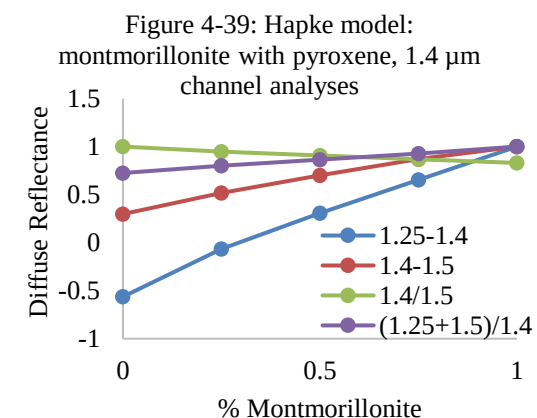
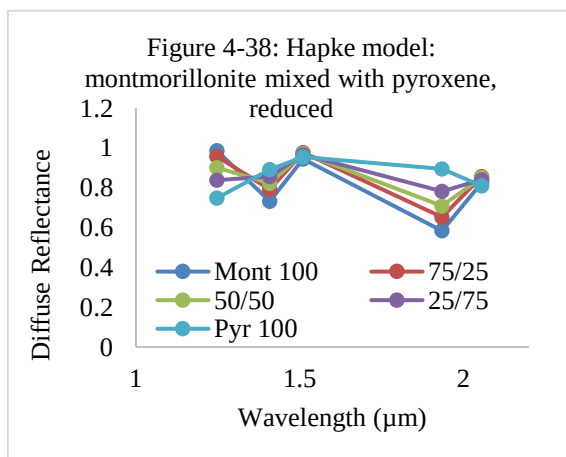
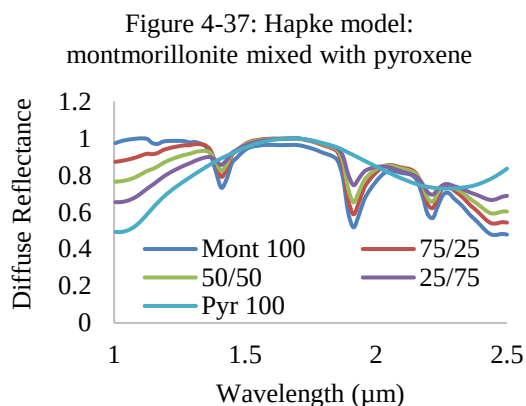
Mineral	Source Optical Constants	USGS ID No.	Particle Fit (μm)	1.4 μm Feature?	1.93 μm Feature?
Gypsum	(Roush et al., 2007)	SU2202	200	No	Yes
Serpentine	Roger Clark via Emery	HS318-3B	100	Yes	Yes
Illite	Roger Clark via Emery	W1R1Ba	10	Yes	No
Kaolinite	Roger Clark via Emery	CM3	10	Yes	Yes
Saponite	Roger Clark Josh Emery	SapCa-1	50	Yes	Yes
Montmorillonite	(Poulet et al., 2008)	CM26	200	Yes	Yes

Each of the minerals were mixed individually with both pyroxene and palagonite. The mixing ratios were pure mineral (100/0) and ratios of 75/25, 50/50, and 25/75. These were modelled in the Emery Hapke widget with the particle size as indicated in Table 4-4 and with 100 μm for Palagonite and 500 μm for Pyroxene.

Band ratios and difference analyses were performed according to the methods outlined in Section 4.6 and Table 4-2.

Results

Montmorillonite mixed with pyroxene is provided here as an example of the process



(Figure 4-37). These were converted to the reduced channel values in Figure 4-38. The best results of the channel analyses are shown in Figures 4-39 and 4-40 for the 1.4 μm and 1.93 μm relationships, respectively.

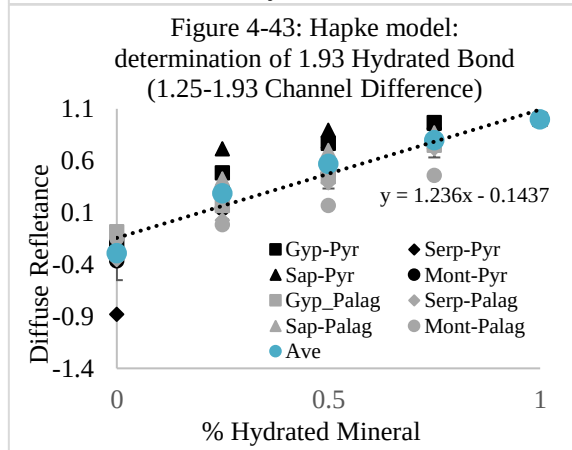
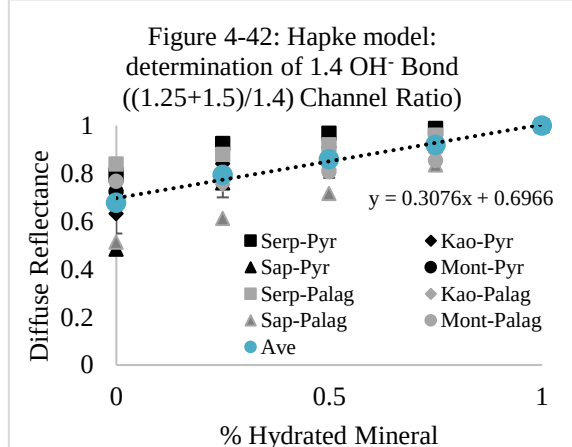
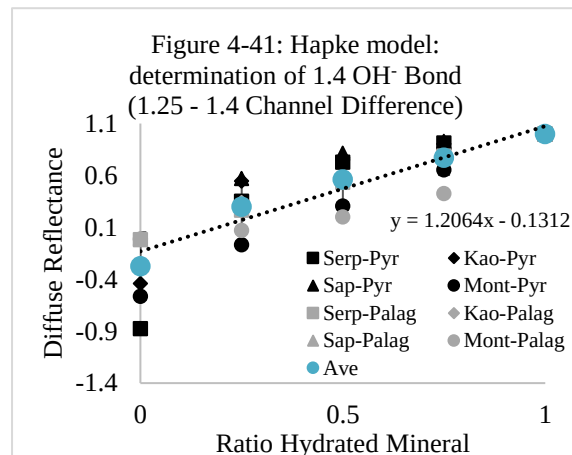
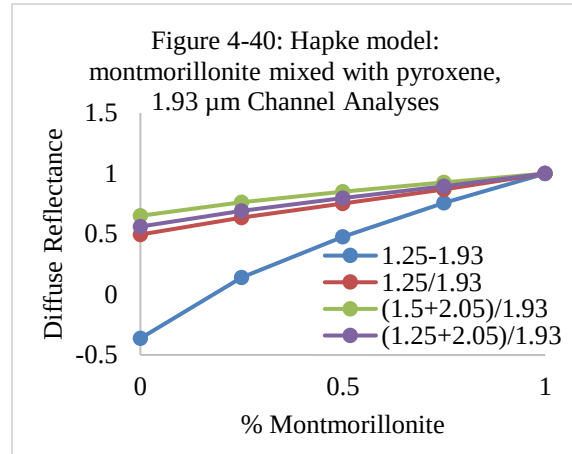
Figures 4-41 shows the data for the 1.25-1.4 μm difference. Figure 4-42 shows the data for the (1.25+1.5)/1.4 μm ratio. The 1.25 – 1.93 μm difference is shown in Figure 4-43.

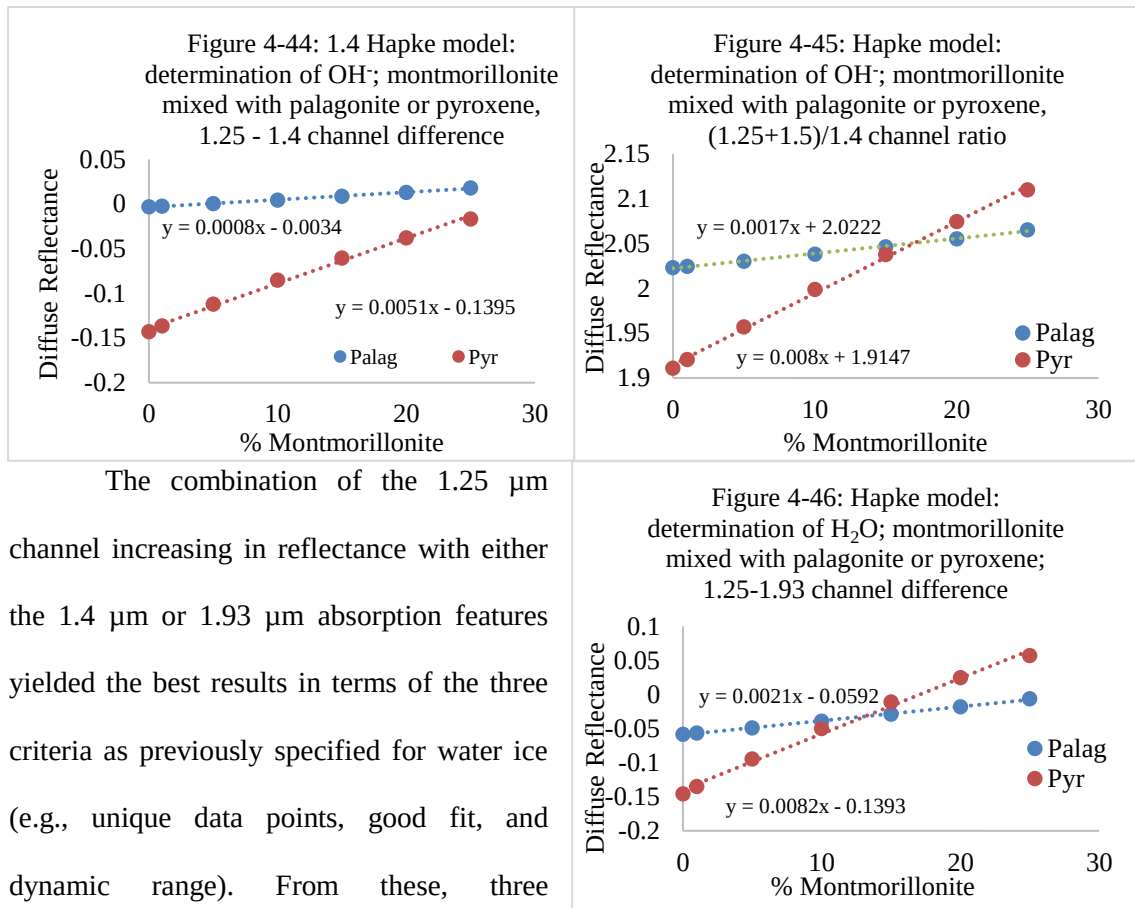
Montmorillonite was evaluated as a separate mineral mixed with pyroxene and palagonite in Figures 4-44 to 4-46.

Discussion

A total of 12 combinations of minerals were run with 5 mixing ratios. Each combination was evaluated individually and then as a group to determine which of the channel relationships were the best.

In Figure 4-37, the pure pyroxene sample shows the typical “S” shape from 1 to 2.5 μm . The 1.4 μm and 1.93 μm absorption features grow as the mixture increases in montmorillonite concentration, while conversely, the 1.25 μm channel increases in reflectance. The 1.5 μm and 2.05 μm channels stay relatively stable with a slight increase in reflectance with increasing concentrations of montmorillonite.





The combination of the 1.25 μ m channel increasing in reflectance with either the 1.4 μ m or 1.93 μ m absorption features yielded the best results in terms of the three criteria as previously specified for water ice (e.g., unique data points, good fit, and dynamic range). From these, three relationships were the best performing. These were broken out individually. For the 1.4 μ m band, it was the 1.25-1.4 μ m channel difference (Fig 4-41), and the (1.25 +1.5)/1.4 μ m ratio (Fig. 4-42). For the 1.93 μ m band, it was the 1.25-1.93 μ m channel difference (Fig. 4-43).

The data are plotted as individual points for each of the 12 mineral combinations for the three relationships. The combination of the points for a channel shows the large variation in the results. These points were averaged and plotted. The purpose of this analysis is just for the positive or negative detection of the two absorption features. These results can serve as a starting point to the analysis of a completely blind sample for the presence of hydrated minerals with either or both OH⁻ or H₂O. The montmorillonite sample had the worst performance in terms of dynamic range due to the high emissivity; therefore, is suggested as the best blind sample proxy for the detection of the two absorption features.

In Figures 4-44 to 4-46, it is clear that the high emissivity of the palagonite as compared to the pyroxene had a significant impact on the reflected energy. This is noted in each of the figures as the fit has a much shallower slope for palagonite to pyroxene. It is recommended to use

the palagonite linear fits as the worst-case performance limitations to determine the existence of the hydration bands at 1.4 μm and 1.93 μm . These will be used to set the instrument performance requirements. Integrated models in Chapter 5 that include the individual component data collected in Chapter 3, will be used to confirm the limits of the method to detect OH^- and H_2O hydration bands.

4.8 Determination of Mixed Mineral Percentage Distribution with Hapke Models

A goal for the instrument is to be able to determine the actual mixture rates of mixed minerals (Table 1-4). As an example of this potential, gypsum was mixed with pyroxene and palagonite (Table 2-7).

Methods

The minerals were mixed and analysed with the methods outlined in Section 4.7. Particles sizes were: 200 μm for gypsum, 100 μm for palagonite, and 500 μm for pyroxene. Channel analyses were performed according to methods outlined in Section 4.6 and Table 4-3.

Results

Figure 4-47 provides mixed spectra results while Figure 4-48 provides normalized values. A summary of the channel relationship results is provided in Table 4-4. The results for the 1.4 μm and 1.93 μm bands are presented in Figures 4-49 and 4-50, respectively.

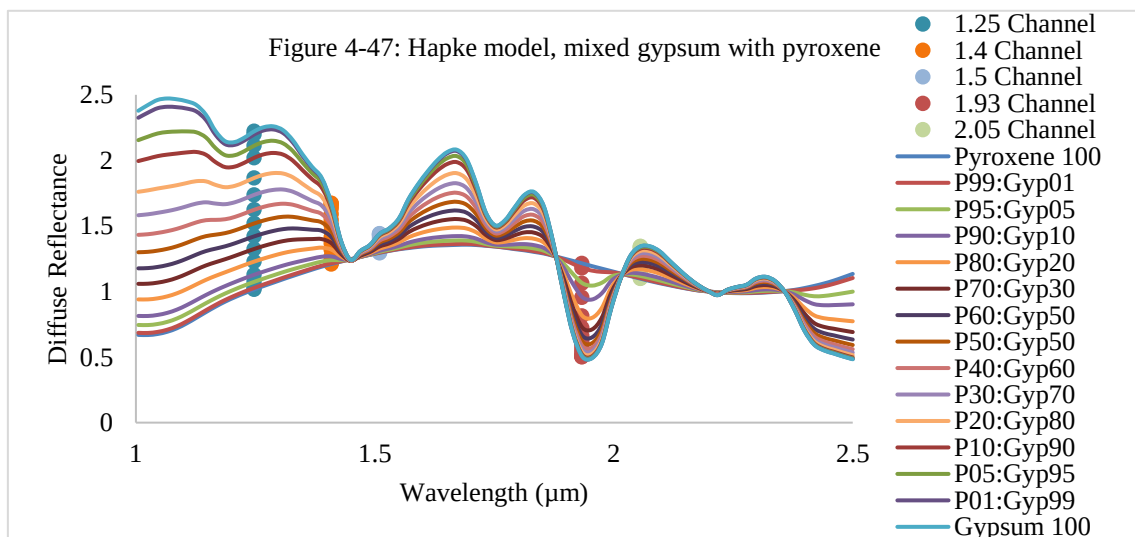


Table 4-5: Channel analysis performance for gypsum with pyroxene and palagonite

	Analysis Channel Combination	Pyroxene			Palagonite		
		1 non-degenerate	2 Good Trend	3 Dynamic Range	1 non-degenerate	2 Good Trend	3 Dynamic Range
Normalized to max series peak value	1.25 – 1.4	✓	✓	✓	✗	✗	-
	1.4 – 1.5	✓	✓	✗	✓	✓	-
	1.25/1.4	✗	✓	✓	✗	✗	✓
	1.4/1.5	✓	✓	-	✓	✓	-
	(1.25+1.5)/1.4	✗	✗	✓	✗	✗	-
	1.25-1.93	✓	✓	✓	✓	✓	✓
	1.4-1.93	✓	✓	✓	✓	✓	✓
	(1.5+2.05)/1.93	✓	✓	✓	-	-	✓
	(1.25+2.05)/1.93	✓	✓	✓	-	✗	✓

Discussion

In general, the palagonite mixtures performed poorer than the mixtures with the pyroxene (Table 4-5). This is attributed to the higher emissivity of the palagonite. Also, the 1.4 μm relationships did not yield good predictive characteristics. This was expected as there is no bound

Figure 4-48: Hapke model (normalized), mixed gypsum with pyroxene, channel values

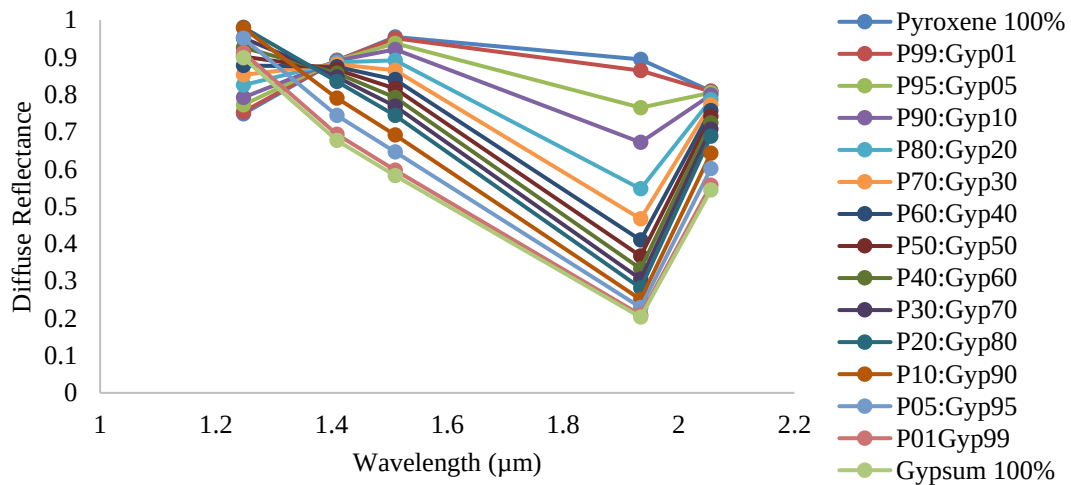


Figure 4-49: Hapke model gypsum mixed with pyroxene or palagonite 1.25-1.93 channel difference

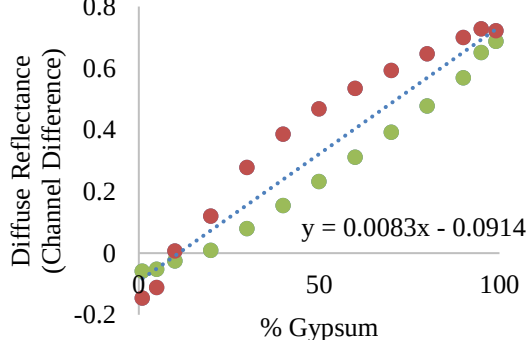
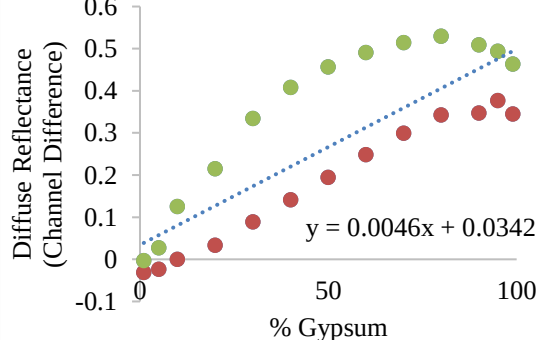


Figure 4-50: Hapke model gypsum mixed with pyroxene or palagonite 1.4-1.93 channel difference



OH⁻ in gypsum or palagonite. This eliminated all but the 1.25- 1.93 μm and 1.4 – 1.93 μm differences (Figure 4-48).

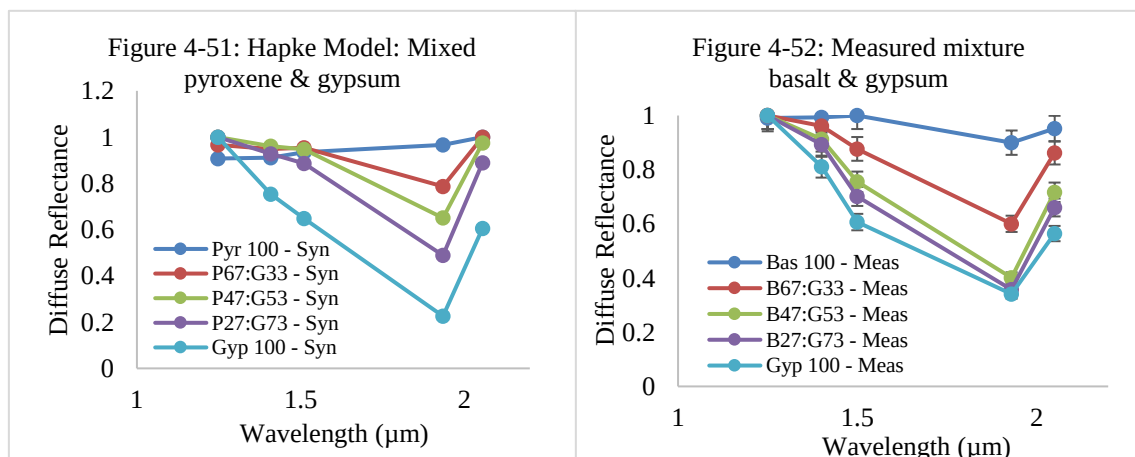
Figures 4-49 and 4-50 indicate that the actual percentage mixtures could be determined from the measured data in these relationships. The palagonite once again has the worst performance; however, there is a good fit in all the four curves and good dynamic range. Grouping the points and taking a linear fit to represent these channels in order to assess a completely blind sample can be done, but the fit is rather poor in both channels. This is, of course, dependent upon the instrument performance that must have sufficient sensitivity to discriminate slight variations in reflected energy.

4.9 Comparison of Hapke models to measured basalt and gypsum mixtures

Synthetic spectra from Hapke models for mixed basalt and gypsum were compared to measured channel radiances. This was previously done for the linear mixed models in section 4.4.

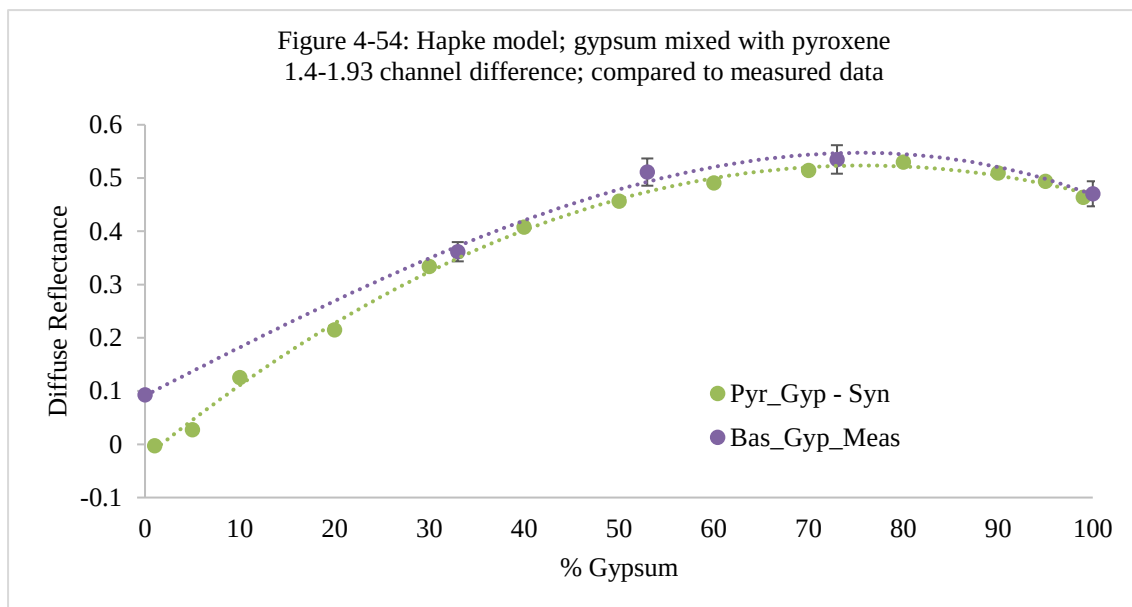
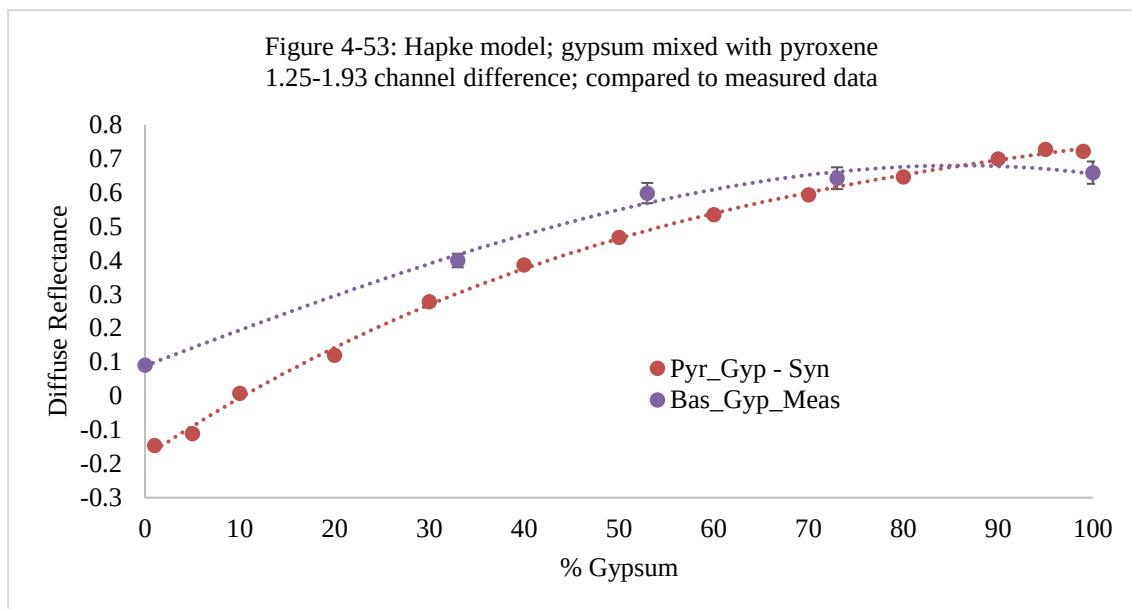
Methods

For the Hapke generated spectra, the minerals were mixed and analysed with the methods outlined in Section 4.7. Pyroxene was used as the proxy to basalt with a particle size of 100 μm while gypsum specifications are listed in Table 4-4. Mixing ratios by volume were per Table 4-1. The measured data were from previous results reported in Section 4.4. From the recommendations in Section 4.8, the values were analysed with the 1.25 – 1.93 μm and 1.4 – 1.93 μm differences.



Results

The Hapke generated spectra are presented in Figure 6-51 while the measured data are presented in Figure 4-52. These values were used to calculate the 1.25 – 1.93 μm and 1.4 – 1.93 μm differences plotted in Figures 4-53 and 4-54, respectively.



Discussion

In Figure 4-51, the 1.93 μm absorption feature is evident, while the 1.4 μm absorption feature is absent. This is correct as neither the gypsum nor the pyroxene have an OH^- bond. The depth of the 1.93 μm feature increases with increasing concentrations of gypsum.

Generally, the measured data have the same shape as the Hapke model generated data (Figure 4-42). The 1.93 μm feature is evident in the measured data while the 1.4 μm feature is absent. Different, however, is that there is a small water feature in the pure basalt end-member at 1.93 μm . This is likely due to absorption of atmospheric water vapour and because this is a terrestrially weathered sample. There is also a slight 1.5 μm water feature showing up in the pure gypsum end-member. This is also likely attributable to the absorption of atmospheric water vapour. Also different is that the 1.93 μm feature saturates much quicker than the Hapke model generated spectra with >50% gypsum resulting in similar diffuse reflectance values.

From Section 4.8, the two most useful channel relationships were the 1.25 – 1.93 μm and 1.4 – 1.93 μm differences (Figures 4-49 and 4-50). These were repeated for this analysis in Figures 4-51 and 4-54. With an assumed $\pm 10\%$ error associated with the Hapke model, and the measured data aligns well with the Hapke data in terms of shape and dynamic range. The 1.25 – 1.93 μm channel relationship had the better dynamic range and no overlapping data points throughout the range, though the fit could be better. The 1.4 – 1.93 μm relationship, on the other hand, had the better fit of the two channel relationships, but was only good up to about 50% Gypsum.

The measured data were a good match to the Hapke calculated data. For the 1.25 – 1.93 μm difference, this was about $\pm 10\%$, while for the 1.4 – 1.93 μm difference, this was within the error bars of 1 standard deviation. This is despite several key forms of error. First, the Hapke data have inherent built in error associated with the measurement and determination of the optical constants. This is accounted for in the 3σ error budget of $\pm 10\%$.

The next key error source is from the measurement of the physical samples. The spectra from the samples measured in this thesis are referenced to KBr powder. This is a stable reference to ratio out atmospheric water vapour that interferes with the spectral measurement, as well as to correlate samples measured at different times. This means that the relative intensities can vary from day to day and instrument to instrument. This was accounted for by normalizing to the maximum series data point.

The next error associated with the measured data is in the samples themselves. Physical samples were selected and characterized to line up as closely as possible to the Hapke optical constants; however, these are not the same physical samples that were used for the generation of the optical constants and there will be differences due to variations in the chemical makeup of the samples and/or weathering. The Morocco basalt is a Ca-pyroxene, but probably not at the same ratio as the Hapke pyroxene optical constants, so assumptions had to be made on the similarities being sufficient for comparison of the physical samples to the Hapke model. This is the same case for the gypsum sample not being the same as the sample used to generate the Hapke model. These were both matched as closely as possible to the Hapke data (Figures 4-17 and 4-20), but there remain unknown errors attributable to the differences in the chemical makeup of the various samples.

Despite these forms of errors, it is evident from Figures 4-53 and -54 that it is possible to discriminate the percent concentration of a hydrated mineral mixed in a non-hydrated mineral. Additional data from external data sets on a Mars mission would help correlate these data and are discussed in Section 5.8.

4.10 Theoretical Models Summary and Recommendations

This chapter started with the introduction of methods of IR thermal emission and reflectance spectroscopy for the measurement of surface temperatures and material discrimination. Thermal and linear and non-linear reflectance models were developed in detail. Methods were presented for the determination of surface temperatures, detection of water ice, and detection of hydrated minerals with OH⁻ with a 1.4 μm absorption feature and water with a 1.93 μm feature. The potential to determine water ice percent concentrations up to 70% and percent concentrations of hydrated minerals mixed with a non-hydrated mineral were presented. Several channel relationships were identified. For water ice, the 1.25 – 1.93 difference was determined to have the best performance, while for hydrated minerals it was the 1.25 – 1.93 and 1.4 – 1.93 differences.

The “spectrometer mode” with assessing all five channels at once is an additional way to allow the detection of the hydration bands and water ice. As shown in Section 4.4 for linear models, a number of combinations of channels can be used for this, or the entire shape. This is a typical approach for Mars that has been used in a number of orbiting and surface instruments including Pancam on ExoMars (Cousins et al., 2010).

A number of errors were identified that are attributable to the measurement of the physical samples and the Hapke modelling. That said, the results in Figures 4-51 and 4-52 and the actual matching of the curves in Figures 4-53 and 4-54 were quite good when all of these errors and separation of data are taken into account. At the very least, the capability for the detection of the water ice and the 1.4 and 1.93 μm absorption bands is entirely viable from these channel relationships. The larger goal of the discrimination of the mixtures remains to be determined as this is controlled by the performance of the integrated system components. This will be developed and specified as part of Chapter 5. Errors are identified and quantified in Section 5.7.

Deconvolving the minerals in the matrix was set as a goal for the thesis because blind samples can be quite difficult to separate and discriminate; however, there are additional data sets that will aid in the discrimination of subsurface materials. This will be presented in Section 5.8.

Chapter 5: Integrated Instrument Performance Models

5.1 Introduction

The objective for this chapter was to prove that the proposed design will have the theoretical capability to meet the science requirements (Table 1-4) leading to final recommendations for the integrated instrument design.

The models developed in Chapter 4 relied on measured spectral data from the various materials and the channels selected for the integrated instrument. A number of channel relationships were tested and several were identified that allow the detection of both water ice and hydrated minerals as well as some limited capability to determine the percentage of either when mixed with two types of typical minerals on the surface of Mars. The capability to measure surface temperature was also demonstrated in both thermal channels. These results were to demonstrate the validity of the method, so the next step is to add in the rest of the known data from each of the components in order to determine the integrated system performance. This will be used to validate that the methods and desired results are obtainable for the proposed integrated instrument.

In this chapter, a theoretical performance model was developed for the integrated instrument in order to determine the capability to measure the full temperature range (Table 1-4) and reflectance by channel (Table 3-9). This model was based on the components specified in Table 3-6 and 3-7. This allowed the establishment of the following parameters for an integrated instrument: Signal to Noise Ratio (SNR), Noise Equivalent Temperature (NET), comparison of the NEP to the expected generated power, determination of the noise voltage, and a theoretical calibration curve of generated voltage to radiance.

5.2 Theoretical integrated instrument performance for thermal channels A and B

A theoretical performance model for thermal channels A and B was developed for the integrated instrument. The performance calculation methods were previously presented in Figure 3-7 (Equations 3-2 to 3-7). Values for D^* , Noise Equivalent Radiance (NER), and Noise Equivalent Power (NEP) for this sensor were previously calculated (Table 3-2), but updated with data from testing (Table 6-5). This update to the performance characteristics also included updates to the expected operational borehole configuration and geometry (described in Sections 1.3 and 1.6). These updated analyses determined the viability of this system prior to integrated breadboard testing under simulated conditions in the laboratory and full-integrated instrument development (Chapter 6).

Methods

This integrated model was based on components specified in Tables 3-6 and 3-7. Because the geometry for a borehole instrument is different than what was used in the component testing, the remaining values were recalculated with an assumed solid angle of the full field of view of the Dexter S25 of $\theta = 35.5^\circ$ and that the detector chip is 4 mm from the surface.

SNR was calculated from Equation 3-8. The integrated radiance was calculated from Equation 4-1. NER was calculated from the integrated radiance divided by the SNR. NET is calculated by Equation 3-1.

The channel power is an estimate of the power generated by the amount of radiance reaching the detector (Equation 5-1). NEP was specified by the manufacturers' datasheet.

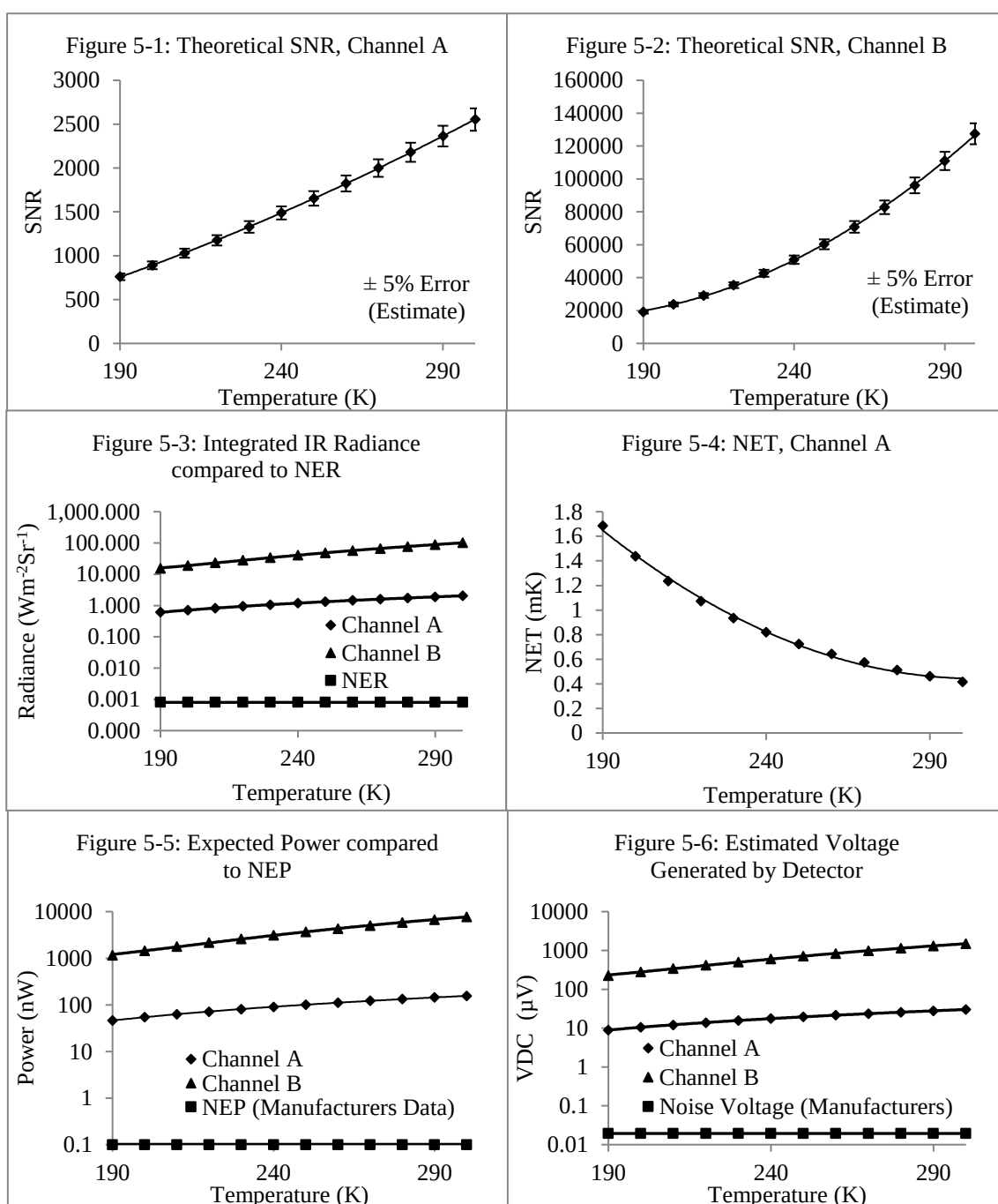
$$\text{Integrated Channel Power} = \text{Integrated Channel Radiance} * a * \Omega \quad \text{Equation 5-1}$$

Where Integrated Channel Radiance is calculated from Equation 4-1, a = active area of the detector element, and Ω = solid angle of the detector to the scene.

The estimated voltage generated by the detector is determined by multiplying the power at each temperature by the number of volts per watt generated by the detector as specified by the manufacturer (Typical 193.9 V/W).

Results

Figures 5-1 and 5-2 plot the SNR. Figure 5-3 compares the integrated IR radiance reaching the detector to the NER. Figure 5-4 shows the NET for integrated borehole instrument, narrow-band configuration. Figure 5-5 compares the expected power at each temperature to the NEP. Figure 5-6 provides the results of this calculation for Channels A and B and compared to the Noise Voltage as specified by the manufacturer of $0.019\ \mu\text{V}$. Figures 5-7 and 5-8 show the results for these plots for Channels A and B, respectively. A summary is provided in Table 5-1.



Discussion

Channel A is the narrowband channel and includes an external narrow band filter with a band pass centred at 25.2 μm (396 cm^{-1}), while Channel B is the wideband channel and does not have any additional external filter beyond the detector

Table 5-1: Calculated Performance Values

Parameter (Channel)		Value
SNR	A	750 to 2550
	B	2×10^4 to 1.2×10^5
NER ($\text{Wm}^{-2}\text{Sr}^{-1}(\text{cm}^{-1})^{-1}$)	A	0.61
	B	15.32
NET (mK)	A	0.4 to 1.7
Channel Power (nW)	A	46
	B	1164

window. Channel A with the narrowband filter represents the worst-case performance. These were all calculated assuming an integration time of 1 s.

Signal to Noise Ratio

The SNR increases with temperature because the thermal IR radiation emission increases with temperature. The removal of the narrow-band filter for Channel B allowed significantly more energy to reach the detector.

Noise Equivalent Radiance

In the thermal channels, the detector measures the energy emitted from the surface, or the integrated radiance. The NER is an estimate of the minimum amount of radiance that can be detected and distinguished by the detector after passing through any filters or windows. If the measured radiance is too close to the NER, it may mean that the instrument is not sensitive enough for the application or that the geometry will need to be changed to increase the SNR. The updated testing of the instrument prototype in Section 6.4 resulted in an $\text{NER} = 0.0007\text{ Wm}^{-2}\text{Sr}^{-1}(\text{cm}^{-1})^{-1}$ (Table 6-5). The calculated radiance reaching the detectors was 760 and 19,000 times higher than the NER for Channels A and B, respectively.

Noise Equivalent Temperature

The next important calculation is for the determination of the Noise Equivalent Temperature (NET), which is the signal noise, converted to a temperature value (Equation 3-1). The calculations for both channels was well below the proposed instrument performance requirement of $\pm 3\text{ K}$ (Table 3-8).

Channel Power compared to NEP

This updated calculation takes into account the borehole configuration (as described in Section 1.3 and 1.6). The increased solid angle significantly improves the expected power compared to the clean room testing. The calculated values for Channels A and B were 463 and 11,644 times higher than the manufacturers NEP of 0.1 nW, respectively.

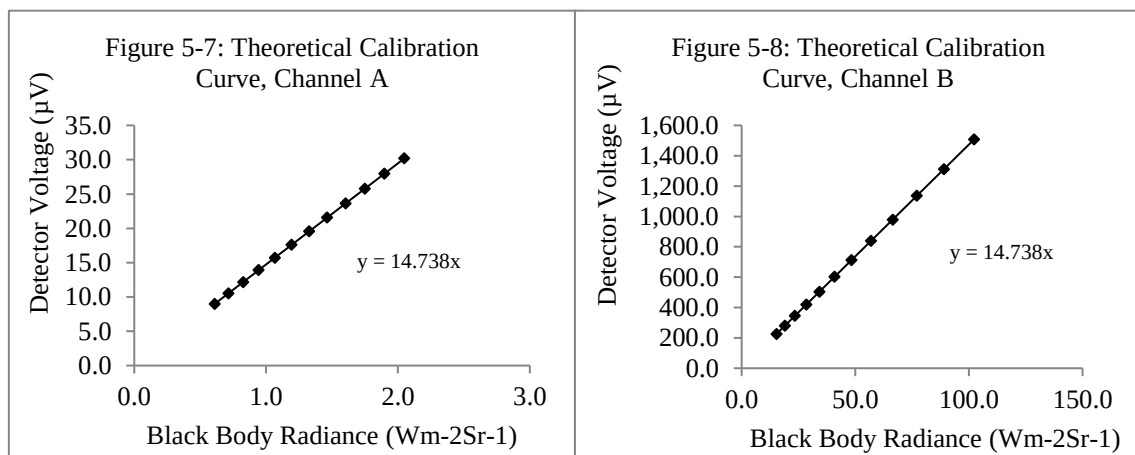
Estimated Generated Voltage to Noise Voltage

The conversion of the channel power to voltage is the last important performance characteristic. The generated voltage is the ultimate measured value. This is an estimate of the voltage that should be generated by the detector for a given scene temperature. It must be sufficiently higher than the manufacturers' specification of the Noise Voltage.

The increased solid angle of the borehole configuration significantly improves the expected generated voltage as compared to the clean room testing and was more than 460 and 11,600 times higher than the manufacturers Noise Voltage for Channels A and B, respectively.

Thermal Calibration Curve and Summary

The overall performance of the thermal channels can be modelled with a theoretical calibration curve plotting the estimated detector voltage generated against the black body radiance. If the previous calculations are correct for these parameters, this plot will yield a linear fit. Figures 5-7 and 5-8 show the results for these plots for Channels A and B, respectively. As expected, the plot of the estimated detector voltage against the radiance results in a linear fit. The equation of the linear fit is the same in both channels. This is also expected, because the fit is a function of the detector performance that is the same in both channels. The amount of energy



reaching the detector is dependent upon the geometry and the window/filter combination. The geometry is the same for both channels, while Channel A has the additional 25.2 μm filter. Therefore, the only difference will be the filter attenuation in Channel A which results in a linear reduction in the generated voltage. There are assumptions and errors with these results that are discussed in Section 5.7. For this chapter, these have been reasonable assumptions; however, a true calibration curve will have to be generated for the as built instrument and tested in a simulated environment in a fixed geometry with materials with known emissivity. This is accomplished in Chapter 6.

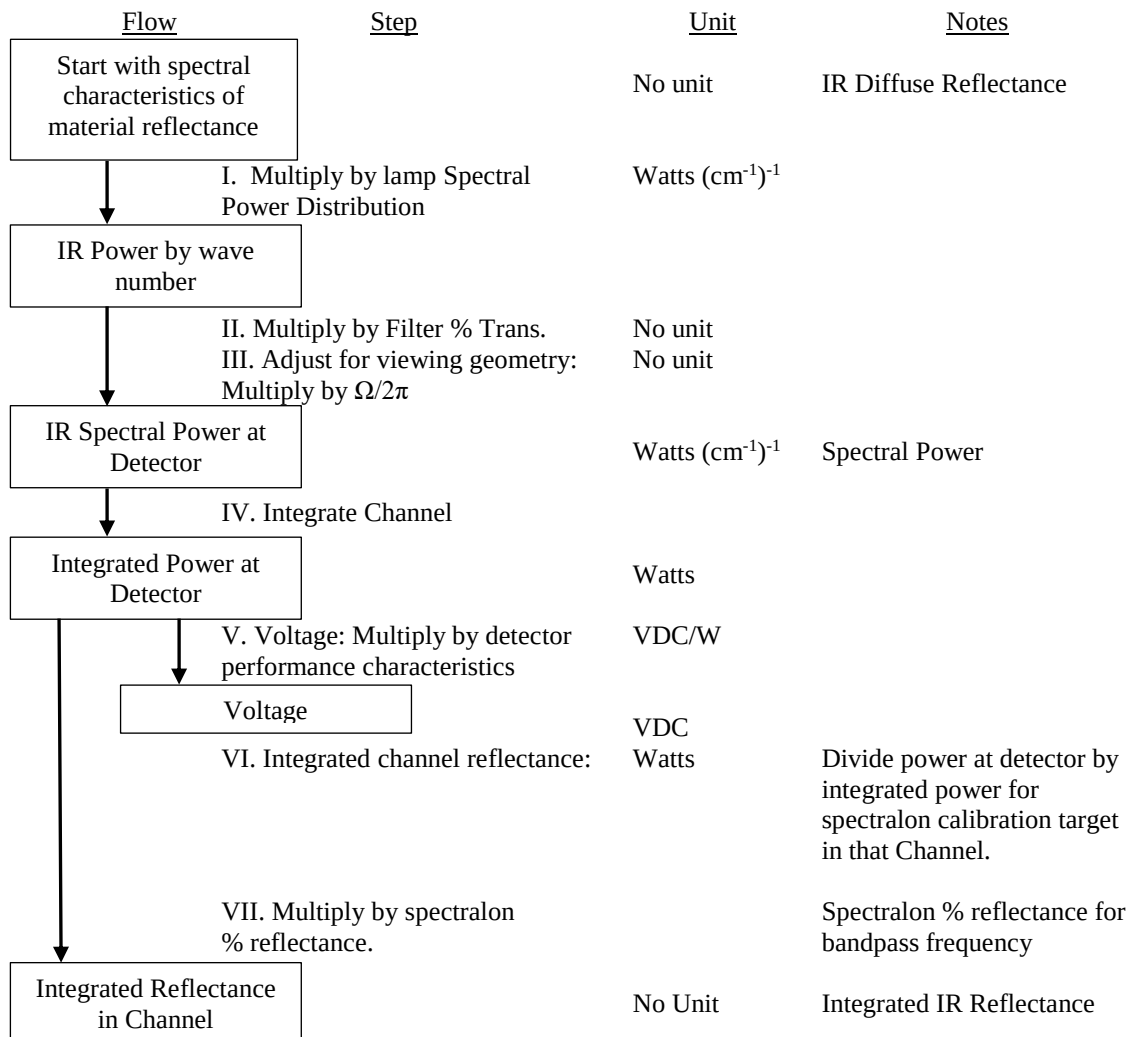
5.3: Method for the calculation of IR integrated channel reflectance and power

The theoretical performance calculations for an IR reflectance filter radiometer are outlined in the flow chart in Figure 5-9.

The geometry was specified in section 5.2. Angle θ is defined by the geometrical cone of light on the surface produced by the design of the LED lamp and is set from each of the manufacturers' data sheet. Because the detector is very close to the surface in the expected bore-hole design (4 mm), the field of view of the Dexter S25 detector ($74^\circ \times 69^\circ$) is larger than the cone of light on the surface defined by angle θ ; therefore, the angle α is set equal to angle θ . This is used to calculate the solid angle Ω of the system. This will be the same Ω that is utilized in the integrated instrument calculations for the thermal and reflectance channels (Figure 3-7).

It is assumed that the surface is Lambertian and that the light from the source is uniformly reflected from the surface in all directions. The calculation of spectral power by frequency must be adjusted for diffuse reflectance. A simplified method for accounting for this is to adjust the amount of reflected light reaching the detector by dividing the solid angle of the detector (in the borehole configuration) by 2π that represents the hemi-sphere of all reflected angles above the surface.

Figure 5-9: Calculation of Channel Power (Power Method)



5.4 Theoretical Instrument Performance for Individual Reflectance Channels

The reflected radiance, power, and voltage were calculated for the five reflectance channels and compared to the NER, NEP, and Noise Voltage in order to determine if the expected performance of the integrated instrument is sensitive enough to detect and discriminate materials.

The detector voltage is directly correlated to the total energy reaching it. This is dependent upon the amount of forward optical power generated by the LED source, the material reflectance properties, and the transmission characteristics of the filter and detector window. This will be different for each channel because a different source is used for each one. Each has different forward optical power values as well as different reflectance properties of the materials within that frequency response range. The capability for the detector to measure this energy requires that

this integrated power is significantly higher than the detector Noise Equivalent Power (NEP), which translates into the Signal to Noise Ratio (SNR).

The integrated channel radiance was calculated and plotted against the original mineral spectral radiances. The SNR and noise voltage represent the detection and discrimination limits for hydrated minerals and water ice for the integrated instrument.

Methods

All calculations were run according to flow chart in Figure 5-9. The calculations were first run for the USGS hematite (FE2602) and Saponite (SapCa-1) samples to confirm that the integrated instrument channel calculations line up with the correct features in the mineral spectral. These were normalized to the integrated power for Spectralon (a calibration standard with a diffuse reflectance of ~98%) and compared to the detector manufacturers specified NEP of 0.1 nW. All calculations assumed a 1 s integration time.

This was then expanded to the 12 minerals collected and characterized in Chapter 2. These mineral spectra are used for the analysis of comparing the predicted result to the reflectance for each sample in each channel.

Predicted reflectance were compared to the channel average reflectance and peak average for each sample. The channel average reflectance is the average reflectance with the range of $\pm 0.5\%$ around the channel peak transmission (e.g., $\pm 0.5\%$ around 1.25 μm , etc.). The average peak reflectance is the average reflectance with the range of ± 0.05 reflectance around the peak transmission (e.g., for 1.25

μm , the range would be from 1.20 to 1.30 μm). These three were mapped to show the differences that band-pass widths would have on the predicted performance of the instrument. The ideal

Table 5-2 Forward Model Non-hydrated USGS minerals

Class	Mineral	USGS Samples (ID)	Mineral Type
Ferric Oxide	Chromite	HS281.3B	Ferric oxide
	Hematite	FE2602	Ferric oxide
	Ilmenite	HS231.3B	Ferric oxide
	Maghemite	GDS81	Ferric oxide
	Magnetite	HS195.3B	Ferric oxide
Carbonate	Calcite	GDS304	Carbonate
Other Non-Hydrated	Albite	GDS30	Tectosilicate
	Anhydrite	GDS42	Sulphate
	Augite	WS588	Inosilicate
	Labradorite	HS17.3B	Tectosilicate
	Olivine	GDS790.a	Nesosilicate
	Pyroxene	HS119.3B	Inosilicate
	Quartz	GDS31	Tectosilicate

case is that the bandpass is at the exact absorption peak. This is obviously not possible with a filter, so it is important to consider how the width of the band based on the average transmission across the band and for a range around the peak compares to the peak absorption.

This was finally applied to a large number of minerals from the USGS database to determine the individual channel detection limits. A total of 31 minerals were identified from the evaluation of the USGS spectral database. These were separated into non-hydrated and hydrated minerals (Tables 5-2 and 5-3, respectively). These spectra were used to

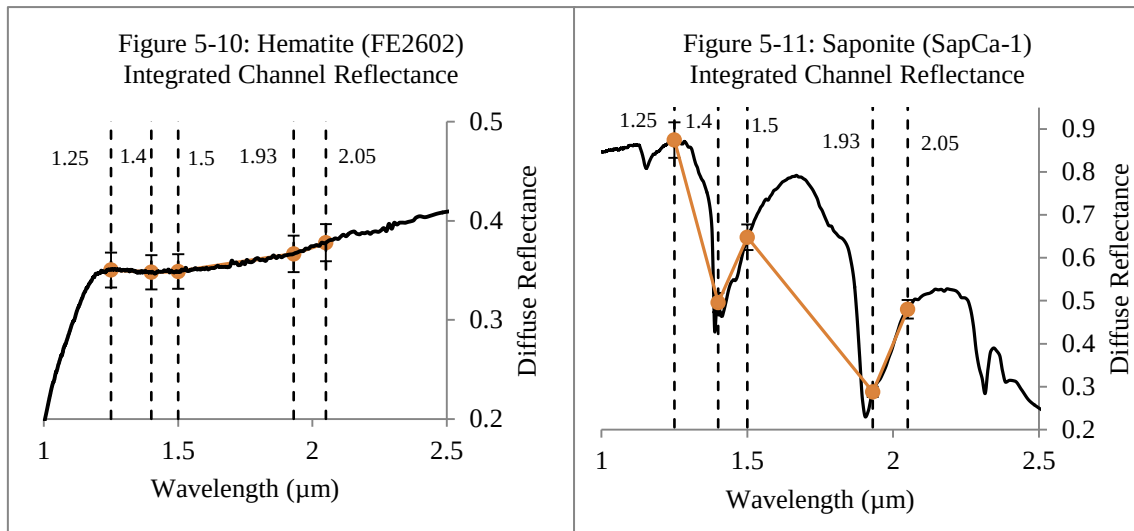
Table 5-3: Forward Model Hydrated USGS minerals

Class	Mineral	USGS Samples (ID)	Mineral Type and Hydration Type
Phyllosilicate	Chlorite	HS179.3B	Phyllosilicate; OH ⁻
	Halloysite	CM13	Phyllosilicate; OH ⁻
	Illite	IL101	Phyllosilicate; OH ⁻ & H ₂ O
	Kaolinite	CM3	Phyllosilicate; OH ⁻
	Kierserite	KIEDE1.a	Phyllosilicate; H ₂ O
	Montmorillonite	CM20	Phyllosilicate; OH ⁻ & H ₂ O
	Muscovite	GDS107	Phyllosilicate; OH ⁻
	Nontronite	NG-1.a	Phyllosilicate; H ₂ O
	Prehnite	GDS613.B	Phyllosilicate; OH ⁻
	Saponite	SapCa-1	Phyllosilicate; OH ⁻ & H ₂ O
Sulphate	Serpentine	HS381.4B	Phyllosilicate; OH ⁻
	Alunite	AL706	Sulphate; OH ⁻
	Bassanite	GDS145	Sulphate; H ₂ O
	Coquimbite	GDS22	Sulphate; H ₂ O
	Epsomite	GDS149	Sulphate; H ₂ O
	Gypsum	SU2202	Sulphate; H ₂ O
Zeolite (Opaline Si)	Jarosite	GDS24	Sulphate; OH ⁻
	Analcime	GDS1	Tectosilicate; H ₂ O
Other Hydrated	Opal	WS732	Tectosilicate; H ₂ O
	Ferrihydrite	GDS75	Ferric Oxide; H ₂ O
	Goethite	GDS134	Hydroxide; OH ⁻

expand the set of instrument performance calculations. The calculations included the power generated compared to the Noise Equivalent Power, and SNR in each channel by mineral.

Results

The results from the basic analysis are presented in Figure 5-10, and 5-11 for Hematite and Saponite, respectively. The results for the comparison of predicted results to the sample reflectance in each channel are presented in Figure 5-12 for the 1.93 μm channel. The other channels are presented in Appendix Figures A-1 to A-4. Figure 5-13 provides the results of this analysis for pure water ice. Figure 5-15 and 5-16 provide examples of the integrated power calculated for each channel for Hematite and Saponite, respectively.



Discussion

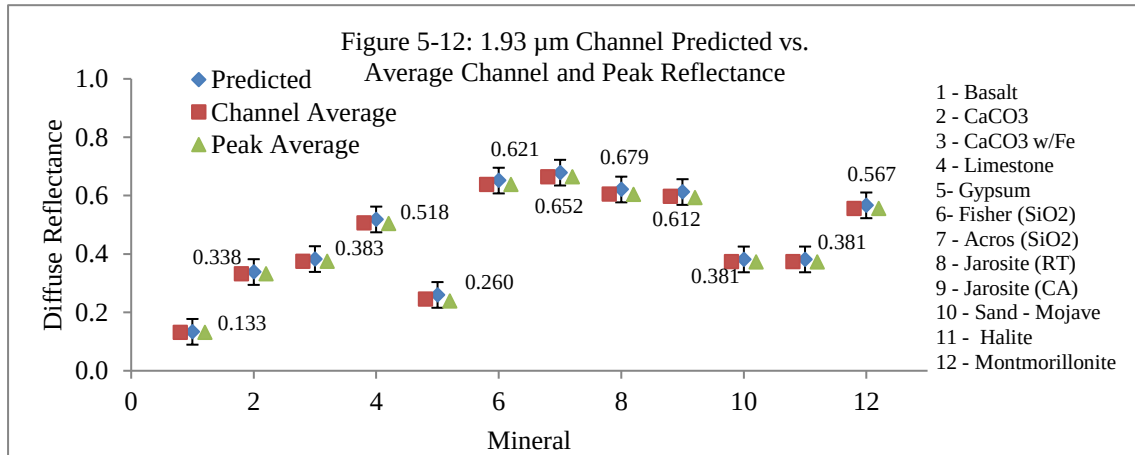
Basic integrated system calculations compared to mineral spectra

The integrated system reflectance was calculated for five channels for hematite and saponite in Figures 5-10 and 5-11, respectively. These values are shown as circles connected by straight lines. The results are the same as the previous calculations shown in Figures 4-4 and 4-5, but have the addition of a system error of $\pm 6.1\%$ (Table 6-9). The results for these two samples confirm the validity of the updated methods to include the system component data as part of the integrated system model. The next step is to expand the data set to additional minerals including those that were collected for testing as part of this thesis from Chapter 2 and the additional minerals from the USGS spectral data set.

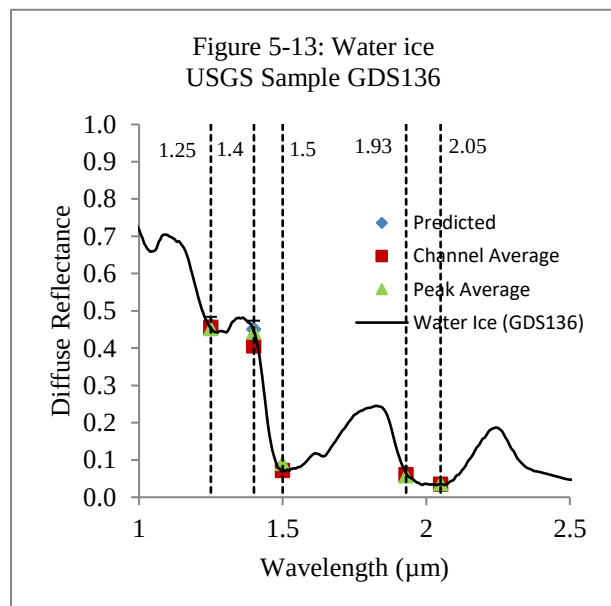
Methods applied to collected minerals

Figure 5-12 plots the results of the 1.93 μm channel for the 12 minerals. The other four channels are provided in Appendix Figures A-1 to A-4. These charts plot the predicted performance with $\pm 5\%$ error against the channel average and peak average for each of the minerals in each channel. A calculated error from the standard deviation of the reflectance values within the bandpass for the channel average and peak average was typically 0.02-0.05%, and not included in the figures (too small to see).

For all of the samples in each of the 5 channels, the predicted value with $\pm 5\%$ error falls within the range of the average and peak average channel values. These are plotted to demonstrate that the predicted value that includes all of the component performance data as part of the calculation is reasonable.



There is variation from one calculation method to the next (e.g., predicted vs. channel average vs. channel peak). This is most directly dependent upon the variation of the spectral response within the transmission range of the filters. If the spectral response of a mineral is flat across the filter transmission frequencies, then the variation will be very low. If; however, there is a significant change in the spectral response of the mineral in the bandpass, then the variation can be much larger. This is demonstrated in Figure 5-13 for pure water ice. In the 1.25, 1.5, 1.93, and 2.05 μm channels, there is little variation in the spectral response, and the different methods have very similar results. The 1.4 μm , on the other hand, has a significant change in the spectral response (Figure 5-14). This results in the channel average being significantly lower than the other two methods. This is because there is a steep drop in the spectral response of water ice from 1.4-1.5 μm that has the effect of lowering the channel average. The predicted value with $\pm 5\%$ error; however, still aligns with the water ice spectra at 1.4

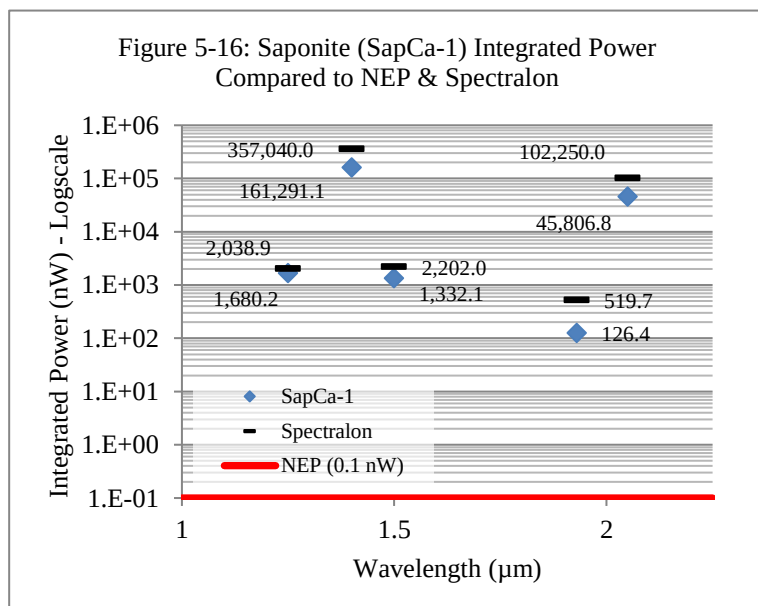
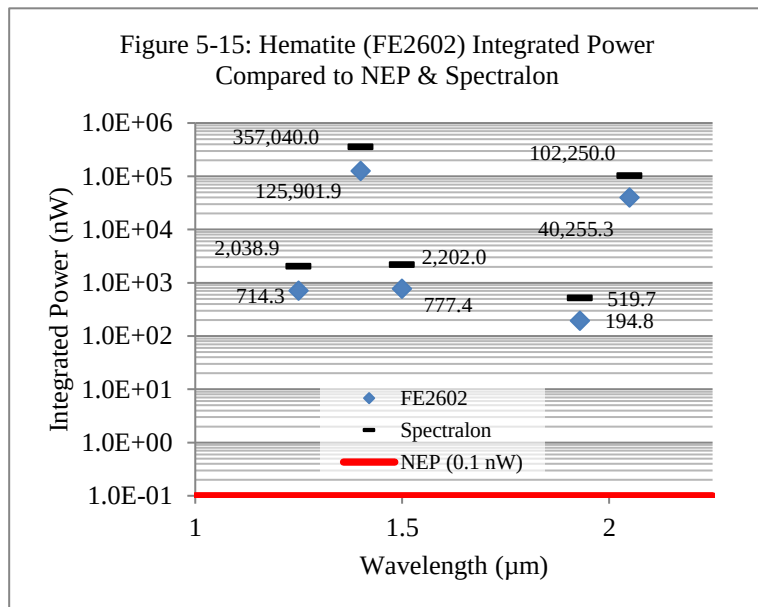
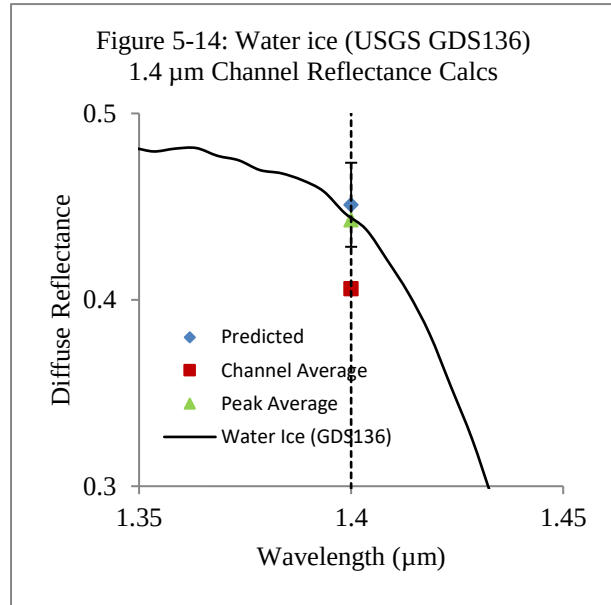


μm , which is the important point for the detection of water ice.

Integrated Power, Noise Equivalent Power and Signal to Noise Ratio Analysis

The channel detection limits were evaluated with the minerals from Tables 5-2 and 5-3. Hematite and saponite are provided as examples in Figures 5-15 and 5-16.

In each channel for both minerals, the integrated power is lower than the Spectralon calculated power. This is expected as the Spectralon has an estimated 98% reflectance across the 1 – 2.5 μm range, and should be significantly higher than the reflected energy of a pure mineral. The integrated power for Spectralon was about 3 times the integrated power reflected off the hematite. For Saponite, the difference ranged from nearly the same in the 1.25 μm channel to >3x in the 1.93 μm channel. This



is because saponite is highly reflective in the 1.25 μm channel, but absorbs in 1.93 μm .

The other important aspect to these two examples is that the integrated power for all channels for both minerals is significantly higher than the detector NEP. The lowest of the values was for the 1.93 μm value for Saponite, which was still 1264x the NEP. This manufacturers' NEP was based off their test configuration. It is assumed here that the 4 magnitudes of performance indicates that the detector should be able to discriminate these reflectance.

The full results are provided in Appendix C, Instrument Power Calculations for the USGS Minerals from Tables 5-2 and 5-3, and Appendix Tables B-3 and B-4. The lowest power values for all of the minerals was in the 1.93 μm channel for Opal, which has a reflectance of 2.6% and the lowest SNR ratio of 140. The typical values of this calculation were in the several thousand. This indicates that the instrument, barring other noise sources, should have the capability to measure these low levels of reflectance with good accuracy.

Summary and recommendations

For pure minerals, the predicted response of the integrated system in each channel was within performance expectations. It should be noted that the filters could have a significant impact on this performance if the transmission range is too wide and includes variations in the material spectral response. These types of errors should be considered when performing the channel relationship analysis to detect and discriminate mixed minerals and water ice.

5.5 Integrated system calculations for Hapke model mixed spectra

The Hapke models developed in Chapter 4 mixed water ice with pyroxene and palagonite and mixed hydrated with non-hydrated minerals. Channel relationships were then developed that could be used to detect and discriminate water ice and hydrated minerals in these general surface materials. In Section 5.4, these generated spectra were used to determine the expected channel power generated from the measurement of pure materials.

The next step is to generate the expected channel power generated from the Hapke mixed mineral spectra to determine if the integrated system performance will be sufficient to both detect and discriminate water ice and hydrated minerals mixed with non-hydrated minerals. Integrated system calculations were developed to match the Hapke generated spectra from Chapter 4 for water ice mixed with pyroxene and palagonite, gypsum with basalt, and montmorillonite with palagonite.

The reflectance values were used to confirm the results of the previous channel analyses in Chapter 4 for water ice mixed with pyroxene. These power and SNR values were used to evaluate the capability of the integrated system to perform these analyses.

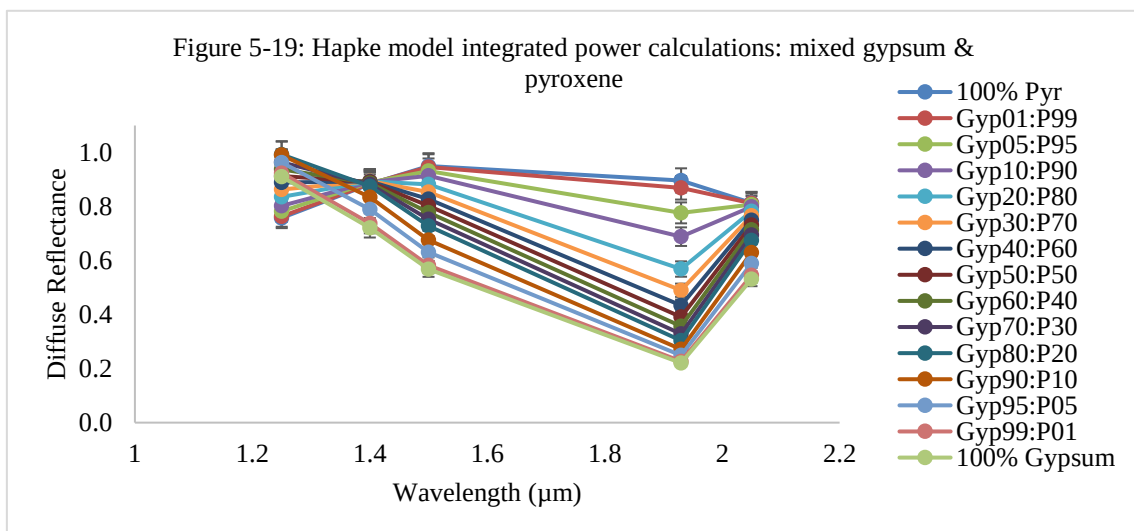
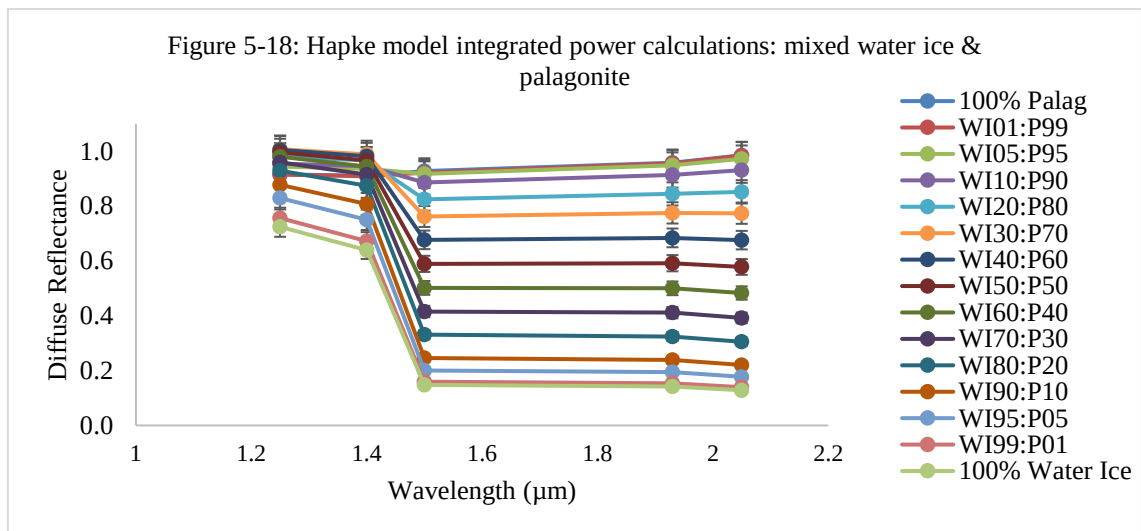
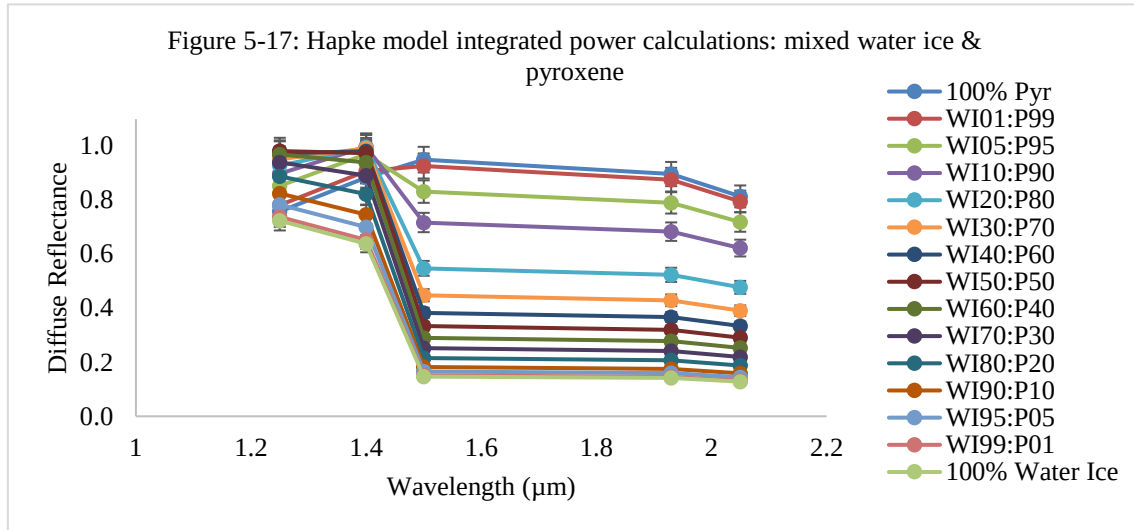
Methods

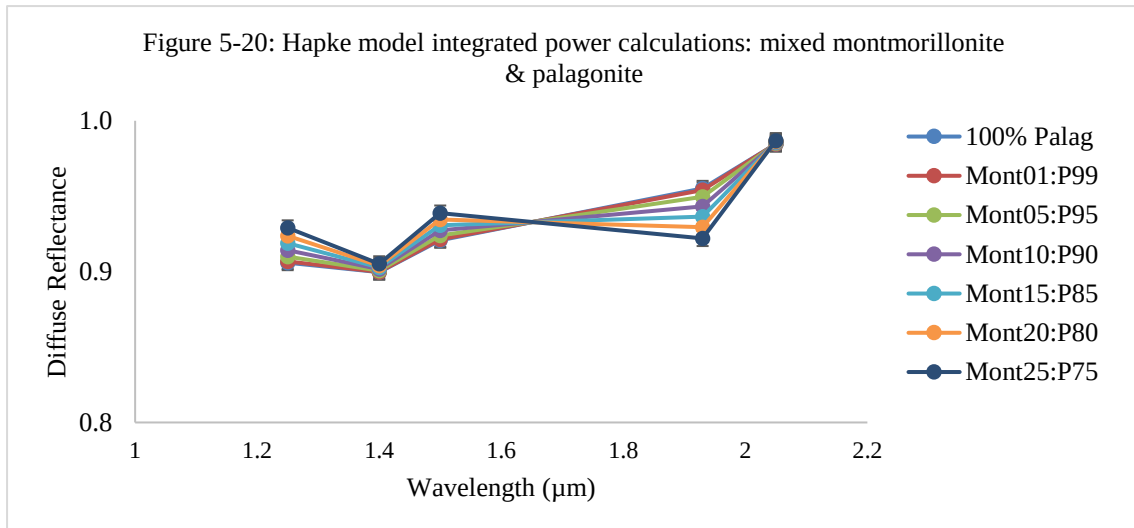
All calculations were run according to the flow chart in Figure 5-9. The Hapke generated spectra for water ice mixed with pyroxene and palagonite (Section 4.6), for gypsum mixed with basalt (Section 4.7), and montmorillonite mixed with palagonite (Section 4.7) were used as the basis for these calculations. Mixture rates were per the referenced sections. The calculations included the power generated compared to the Noise Equivalent Power, and SNR in each channel by mineral, and the integrated channel reflectance.

Results

The resulting calculated reflectance are shown in Figure 5-17 for water ice mixed with pyroxene, Figure 5-18 for water ice mixed with palagonite, Figure 5-19 for gypsum mixed with basalt, and Figure 5-20 for montmorillonite mixed with palagonite.

The integrated power values for each channel and mixture are provided in Appendix Table B-3 and ranged from 75.3 to 168.9 nW. The SNR calculations are provided in Appendix Table B-4 and ranged from 753 to 1689.





Discussion

Water ice & pyroxene

The results of this updated analysis (Figure 5-17) closely match the results previously determined in Figure 4-25. Minor differences between these two results are due to the addition of the LED frequency power distribution and the spectral transmission characteristics of the filters and detector window.

The integrated power values for each channel and mixture ranged from 75.3 to 168.9 nW, while the SNR from 753 to 1689. The integrated power compared to the NEP is one of the most important data points in the consideration of the expected performance of the instrument. For these calculations, the functional range is assumed to be from 0.1 nW (the NEP) due to internal heating up to 100% diffuse reflectance as the channel maximum.

The channel power should be significantly higher than the NEP as indicated by the SNR. The worst performing channel is the 1.93 μm channel with 100% water ice resulting in an SNR of 753, while the other channels are in the 10^3 to 10^6 range. This is because the 1.93 μm LED had the lowest forward optical power of the set combined with this channel having the highest absorption for pure water ice. It would still appear to be acceptable, as a SNR of at least several hundred is typically considered sufficient for the purpose (Taylor, 2010).

Water ice & palagonite

Evaluation of water ice mixed with palagonite followed the same steps as with pyroxene. Figure 5-18 shows the results of the integrated power expected to be generated from the

measurement of this mixture. Similar to the pyroxene results, these closely match the results of Chapter 4 (data not provided, see example Figures 4-31 to 4-33), with the differences attributed to the same sources (e.g., LED frequency power distribution and spectral transmission characteristics of the filters and detector window).

The 1.93 μm channel was the lowest performing channel. The integrated power analysis resulted in a range from 75.3 nW (100% water ice) to 137.3 nW (100% Palagonite) (data not provided). The power to NEP ratio in the 1.93 μm channel ranged from 753 (100% water) to 1373 (100% palagonite) (data not provided).

Gypsum & pyroxene compared to measured gypsum & basalt

Figure 5-19 shows the results of gypsum mixed with pyroxene. These results closely match the results of Figure 4-48 with the same differences as the previous two analyses.

The 1.93 μm was the lowest performing channel. The integrated power analysis resulted in a range from 75.8 nW (100% gypsum) to 184.8 nW (100% pyroxene) and the SNR in the 1.93 μm channel ranged from 758 (100% gypsum) to 1848 (100% pyroxene) (data not provided).

Montmorillonite and palagonite

Figure 5-20 shows the results of montmorillonite mixed with palagonite. This combination was recommended for further evaluation in Chapter 4 because it had the smallest dynamic range for all of the mixtures considered and would be a good indication of the limits of the integrated system to detect and discriminate the 1.4 and 1.93 μm absorption features. The concentration of Montmorillonite in Palagonite was evaluated from 0 to 25%.

The dynamic range is very limited. Neither the 1.4 nor the 2.05 μm channels have much variation, while the other three channels have some variation. As in the other analyses, the 1.93 μm is the most limited in performance with an integrated power ranging from 137.4 nW (100% palagonite) to 133.9 nW (100% montmorillonite). With the limited mixing range of 0-25% montmorillonite, the expected generated power was from 136.9 to 137.4 nW. This appears to be a poor dynamic range; however, the channel ratio analyses in the next section will determine if it is possible to detect and discriminate this combination.

Section Summary

The power generated in each of the channels was well above the 0.1 nW NEP of the instrument for all the combinations; however, the montmorillonite mixed with palagonite had a poor dynamic range as was previously suggested in Chapter 4. This would indicate that the instrument will be able to both detect and discriminate the majority of the expected mineral combinations. This will have to be confirmed with the ratio and difference analysis in the next section.

5.6 Channel analyses with integrated system data

The channel ratios and differences recommended from Chapter 4 were applied to the mixture calculations from Section 5.5. The 1.25-1.93 difference was recommended in Chapter 4 for water ice mixed with pyroxene and palagonite. The 1.25-1.93 and 1.4-1.93 differences were recommended from Chapter 4 for gypsum/basalt and montmorillonite/palagonite mixtures.

Methods

Data for the individual channel mixtures were calculated in Section 5.5. Methods for the determination of ratios and difference was from Section 4.6 for the water ice mixtures and 4.7 and 4.8 for the gypsum/basalt and montmorillonite/palagonite mixtures. Measured component data was taken from Chapter 3 datasets.

Results

The results for water ice mixed with pyroxene and palagonite are provided in Figures 5-21 and 5-22, respectively. Also plotted in these figures is a 1.4 – 2.05 difference.

The integrated channel calculations for gypsum mixed with basalt/pyroxene are presented in Figures 5-23 and 5-24, respectively. These results are compared to Chapter 4 calculations and the measured component data from Chapter 3.

The integrated power calculations for montmorillonite mixed with palagonite are provided in Figures 5-25 and 5-26 for the 1.25 – 1.4 μm and the 1.25-1.93 μm differences, respectively.

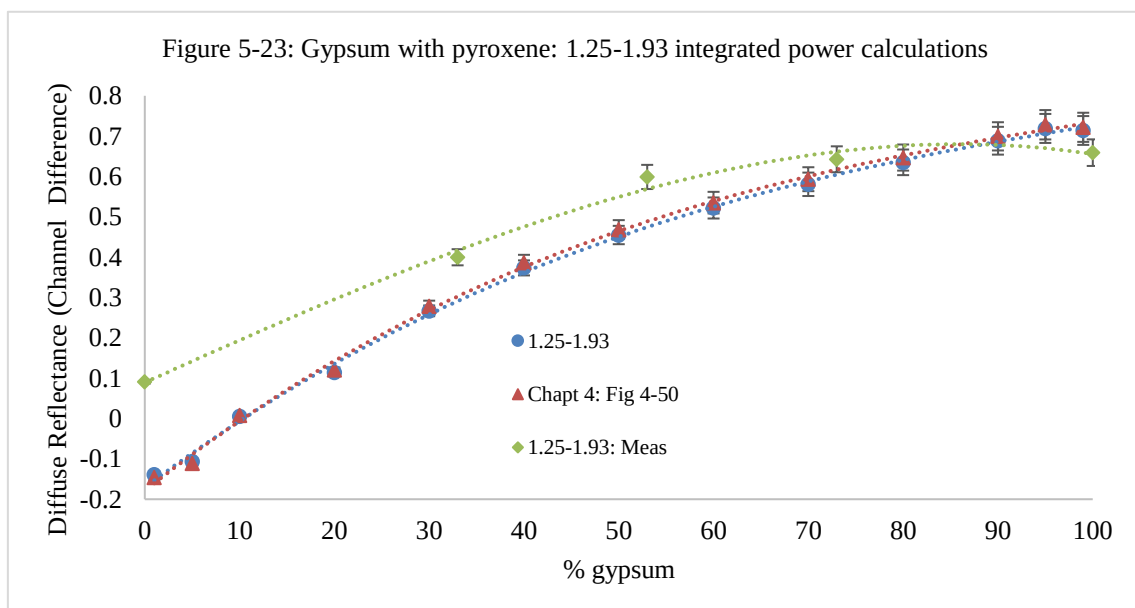
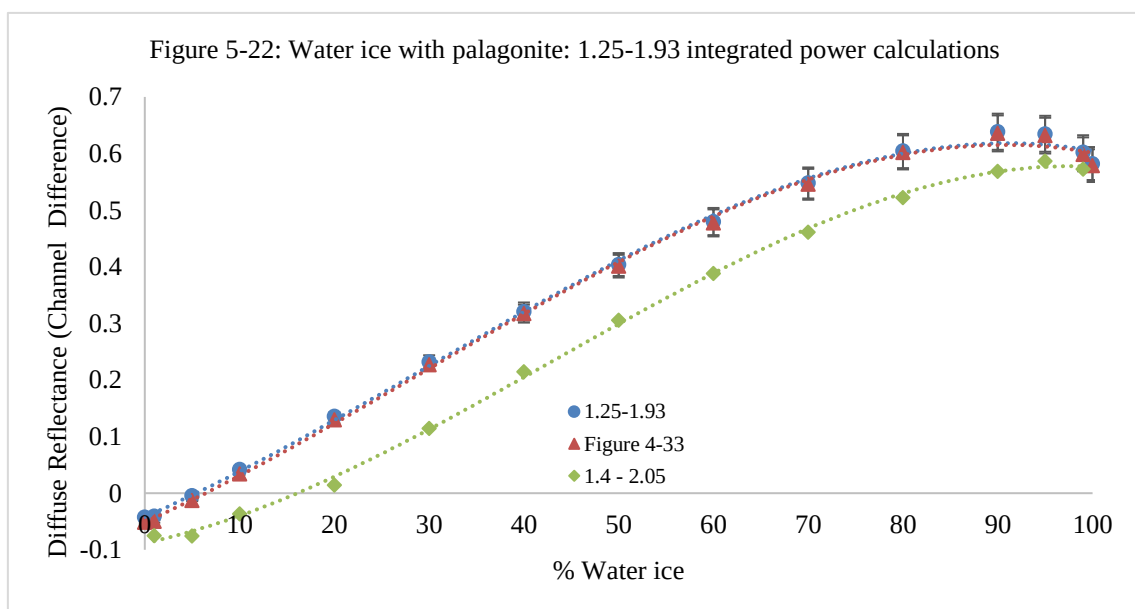
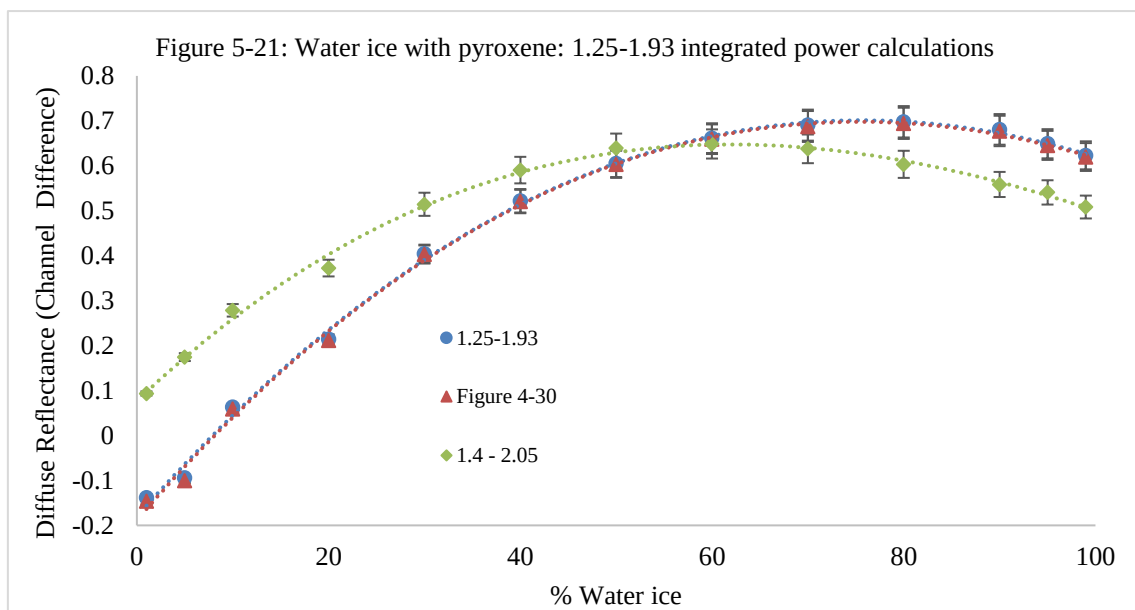


Figure 5-24: Gypsum with pyroxene: 1.4-1.93 integrated power calculations

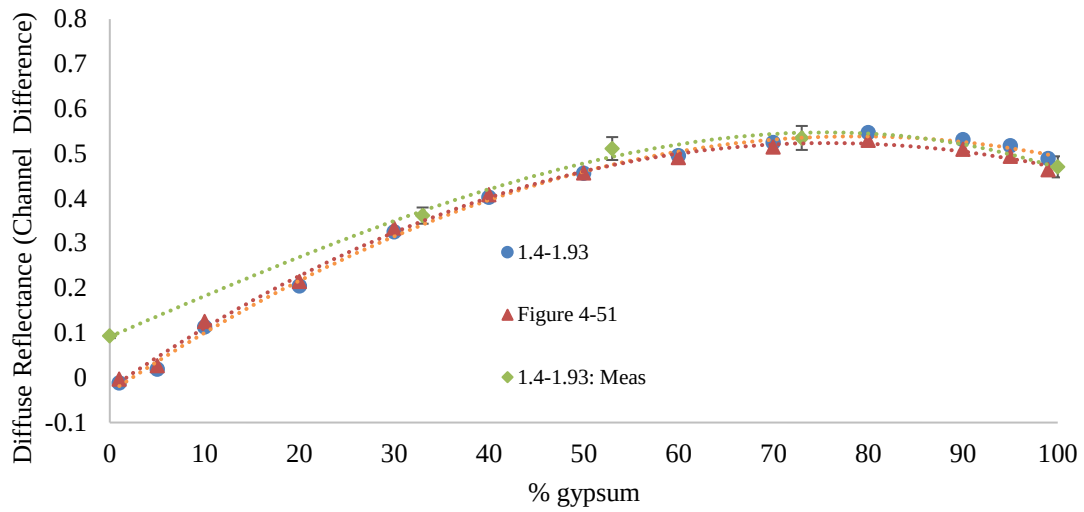


Figure 5-25: Montmorillonite mixed with palagonite: 1.25 - 1.4 integrated power calculations

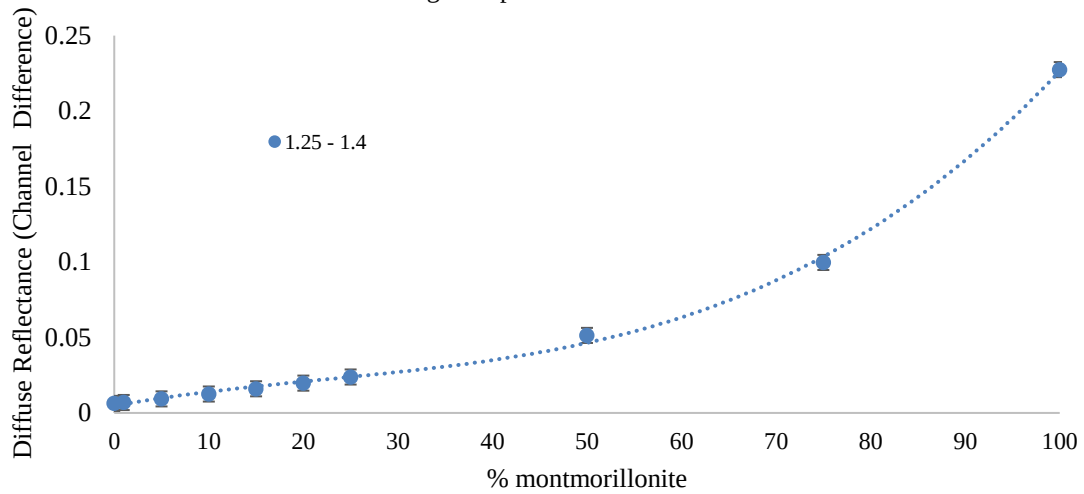
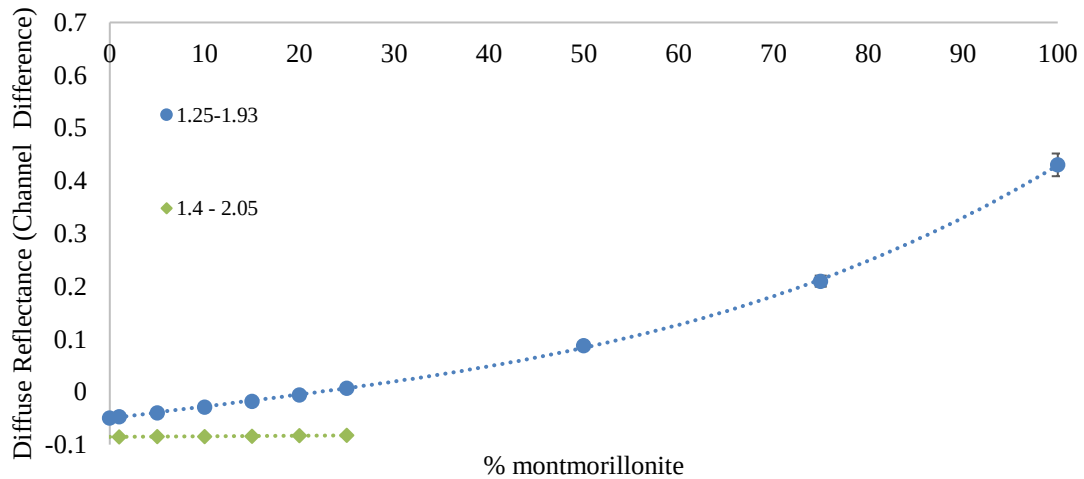


Figure 5-26: Montmorillonite mixed with palagonite: 1.25 - 1.93 integrated power calculations



Discussion

Water ice mixed with pyroxene and palagonite

In both Figures 5-21 and 5-22, the power calculations match the Chapter 4 calculations with differences attributed to the LED spectral power distribution and filter/window transmission characteristics. Figure 5-21 and 5-22 demonstrate that discrimination of water ice mixed with pyroxene or palagonite, respectively is limited to about 60% water ice content for the 1.25 – 1.93 μm difference before it overlaps with values in the upper end. Because the requirement is 1-15% water ice content, this is acceptable. The dynamic response range appears to be sufficient to distinguish the lower end water ice concentrations with these ratios with at least 1% accuracy.

The spectral response of water ice mixed with these two materials is quite different in terms of shape. Pyroxene represents a general surface material found on the surface of Mars, while the palagonite simulates JSC Mars-1 spectra, which is a common material, used for laboratory simulations of general Mars surface materials. Trying to combine the results of these two materials into a single average would result in a significant error, as was shown in Figures 4-41 to 4-43 for hydrated minerals mixed with palagonite and pyroxenes. An operational consideration could be to measure both surface materials and borehole cuttings prior to measurement in a borehole to ensure that the base matrix material is characterized spectrally which will allow a more precise model and calculation for water ice percentages in the borehole.

Gypsum mixed with Basalt

Figures 5-23 and 5-24 demonstrate that the calculations from the two chapters are very similar with the expected differences as discussed in the previous section with water ice mixtures. The results of the comparison to the measured data for the gypsum/basalt mixtures are the same as discussed for Figures 4-53 and 4-54. Summarized here, the measured data compared to the integrated model match is good in terms of general shape and dynamic range, especially for the 1.4-1.93 difference (Figure 5-24) which overlaps well within a $\pm 5\%$ error from $>30\%$ gypsum. Below 30%, the results deviate from the Hapke generated spectra. This is most likely because of the low quantity of gypsum in the sample not truly being an intimate mixture in the physical sample, while the Hapke model assumes an intimate mixture.

Montmorillonite mixed with Palagonite

Figure 5-25 plots the integrated power calculations for montmorillonite mixed with palagonite. This combination represents the worst case performance because of the emissivity of the materials, per the recommendations of Section 4.7. The dynamic range is limited in the <25% concentration range because of the high emissivity of montmorillonite. On the other hand, the 1.25 and 1.4 μm channels have a power to NEP ratio of at least 2×10^4 . This is at least 1,000x better performance than the 1.25 – 1.93 μm difference power to NEP ratio.

Figure 5-26 compares the 1.25-1.93 difference calculations from the integrated power and Chapter 4 values (Figure 4-46). This has more dynamic range in terms of diffuse reflectance values; however, the channel is limited by the performance of the 1.93 μm LED with a power to NEP ratio of 3000. Even with a $\pm 5\%$ error, the device would appear to be able detect the 1.93 μm absorption band with this worst-case combination when the concentration is at least >25%.

Similar to the previous analysis, an understanding of the surface material or borehole cuttings could significantly improve the models and interpretation of borehole data sets.

5.7 Sources of Error

There are a three principal categories of errors. These are 1) Spectral confusion, 2) Analogue material measurement errors, and 3) Radiometric model errors associated with component performance. Some of these will have a numerical value while others will have procedural limitations. The goal of this analysis is to determine the limits of both detection and discrimination and to identify under what conditions and type of materials it will and will not function.

Spectral confusion

Spectral confusion has to do with spectral features that are not consistent with the expected band positions. In most hydrated minerals, the individual element bond positions are within a range such that when they vibrate, the result is an absorption feature at around 1.4 μm for OH^- and from 1.90-1.95 μm for H_2O . There is variation depending on the angle of the bonds,

and in some cases, there can be enough variation that would move the absorption feature out of the range of the instrument design, causing a false negative. Conversely, non-hydrated minerals can have a feature that might cause a false positive, such as the 2 μm feature for pyroxenes.

A detailed analysis of the errors resulting from the concavity of absorption features at 1.4 and 1.93 μm was developed for the 31 pure minerals from the USGS database. The results and proposed corrections are provided in Table 5-4. This is a “yes” or “no” analysis, though some effort is made to determine strong or weak absorbers based on the depth of the absorption features at 1.4 and 1.93 μm . It is assumed that any absorption features of the pure minerals will remain in the same place as they are mixed with other minerals, so that the evaluation of pure minerals is a reasonable approach. This table has both colour coding and written information.

Table 5-4: Error Analysis and Proposed Corrections for Integrated Channel Reflectance

Mineral	USGS Sample #	Chemical Formula	Mineral Contains		Concave Shape at		Correct	Error Mode and Correction			
			OH	H ₂ O	1.4 μm	1.93 μm		+ OH	- OH	+ H ₂ O	- H ₂ O
Albite	GDS30	NaAlSi ₃ O ₈	No	No	-	+	Minor			Shape	
Anhydrite	GDS42	CaSO ₄	No	No	-	++	Minor			Shape	
Augite	WS588	(Ca,Na)(Mg,Fe,Al,Ti)(Si,Al) ₂ O ₆	No	No	-	-	Yes				
Calcite	GDS304	CaCO ₃	No	No	-	-	Yes				
Chromite	HS281.3B	Fe ²⁺ Cr ₂ O ₄	No	No	-	-	Yes				
Hematite	FE2602	alpha-Fe ₂ O ₃	No	No	-	-	Yes				
Ilmenite	HS231.3B	Fe ²⁺ TiO ₃	No	No	-	-	Yes				
Labradorite	HS17.3B	(NaAlSi ₃ CaAl ₂)Si ₂ O ₈	No	No	-	-	Yes				
Maghemite	GDS81	gamma-Fe ₂ O ₃	No	No	-	-	Yes				
Magnetite	HS195.3B	Fe ²⁺ Fe ³⁺ O ₄	No	No	-	-	Yes				
Olivine	GDS70.a	Mg ₂ Si ₄ Fe ₂ SiO ₄ Fo ₉₈	No	No	+	-	Minor	Shape			
Pyroxene	HS119.3B	(Ca,Mg,Fe ²⁺ ,Fe ³⁺ ,Ti,Al) ₂ (Si,Al) ₂ O ₆	No	No	-	-	Yes				
Quartz	GDS31	SiO ₂	No	No	-	-	Yes				
Alunite	AL706	(Na,K)Al ₃ (SO ₄) ₂ (OH) ₆	Yes	No	-	-	Minor		1.5 μm		
Analcmite	GDS1	NaAlSi ₃ O ₈ •H ₂ O	No	Yes	+++	+++	No	+++			
Bassanite	GDS145	2CaSO ₄ •H ₂ O	No	Yes	++	+++	No	++			
Chlorite	HS179.3B	(Mg,Fe) ₃ (Si,Al) ₄ O ₁₀ (OH) ₂ •(Mg,Fe) ₃ (OH) ₆	Yes	Yes	+	+	Yes				
Coquimbite	GDS22	Fe ₂ ³⁺ (SO ₄) ₃ •9H ₂ O	No	Yes	-	+	Minor			Shape	
Epsomite	GDS149	MgSO ₄ •7H ₂ O	No	Yes	-	-	Yes				
Ferrihydrite	GDS75	5Fe ³⁺ O ₃ •9H ₂ O	No	Yes	-	+++	Yes				
Geothite	GDS134	alpha-FeO(OH)	Yes	No	-	+	No		-	Shape	
Gypsum	SU2202	CaSO ₄ •2H ₂ O	No	Yes	-	+++	Yes				
Halloysite	CM13	Al ₂ Si ₂ O ₅ (OH) ₄	Yes	No	+++	++	Minor			Shape	
Illite	IL101	(K,H ₃ O)(Al,Mg,Fe) ₂ (Si,Al) ₄ O ₁₀ [(OH) ₂ •(H ₂ O)]	Yes	Yes	+++	++	Yes				
Jarosite	GDS24	NaFe ³⁺ ₃ (SO ₄) ₂ (OH) ₆	Yes	No	+	-	Minor		1.5 μm		
Kaolinite	CM3	Al ₂ Si ₂ O ₅ (OH) ₄	Yes	No	+++	+	Minor			Shape	
Kierserite	KIEDE1.a	MgSO ₄ •H ₂ O	No	Yes	-	-	Minor				Shape
Montmorillonite	CM20	(Na,Ca) _{0.33} (Al,Mg) ₂ Si ₄ O ₁₀ (OH) ₂ •nH ₂ O	Yes	Yes	-	-	Minor		1.5 μm		2.05 μm
Muscovite	GDS107	KAl ₂ Si ₃ O ₁₀ (OH) ₂	Yes	No	+++	+	Minor			Shape	
Nontronite	NG-1.a	Na _{0.33} Fe ³⁺ ₃ (Si,Al) ₄ O ₁₀ •nH ₂ O	No	Yes	-	+++	Minor				
Opal	WS732	SiO ₂ •nH ₂ O	No	Yes	+	+	Minor	Shape		Shape	
Prehnite	GDS613.B	Ca ₂ Al ₂ Si ₂ O ₁₀ (OH) ₂	Yes	No	-	+	Minor		1.5 μm	Shape	
Saponite	SapCa-1	($\frac{1}{2}$ Ca,Na) _{0.33} (Mg,Fe ²⁺) ₃ (Si,Al) ₄ O ₁₀ (OH) ₂ •4H ₂ O	Yes	Yes	+++	+++	Yes				
Serpentine	HS381.4B	Mg ₃ Si ₂ O ₅ (OH) ₄	Yes	No	++	+	Minor			Shape	

Note: “+” is for weak absorption feature; “++” for medium absorption feature; and “+++” for a strong absorption feature.

The first three columns provide the mineral name, the specific USGS spectra that were analysed for that mineral (sometimes there is more than one available and selection was arbitrary), and the chemical formula. The later allows the determination of the hydration state with OH

and/or H₂O. The next two columns only confirm the hydration type. These are colour coded with purple for “No” and brown for “Yes”, just for visual ease of determining which mineral has what type of hydration or not. The next two columns provided data from the spectra in Appendix C to visually determine absorption features at 1.4 and 1.93 μm . If it has no feature, then a “-” is entered. If it has an absorption feature then it is noted as “+” for a weak absorption, “++” for a medium absorption, and “+++” for a strong absorption. These are further colour coded where green indicates a correct result, red indicates an incorrect result, and yellow indicates a minor error that might be eliminated through further evaluation of the overall shape. The next column confirms if it is correct, incorrect, or a minor error with the same red/yellow/green colour coding. The next four columns provide information on the Error Mode (false positive OH⁻, false negative OH⁻, false positive H₂O, or false negative H₂O). The individual cells in these columns provide a correction method and colour codes if the result can be corrected through further evaluation (green is corrected, red not possible to correct, and yellow remains an uncertain result).

After the corrections, there are three minerals of the 31 that appear to have features that cannot be corrected. Analcime is an H₂O hydrated mineral without OH⁻ in the composition; however, it is absorbing as if it has an OH⁻ bond. Further research in the literature identified an obscure reference to the potential for Al-O-Si bridges to be broken by H⁺ atoms creating a localized OH⁻ group (Bish et al., 2006). Probably, it would not be encountered, but if it is, locally bonded OH⁻ in this mineral should be less likely on Mars since the capacity to form the OH⁻ bonds depends on an aqueous environment, which is not typical of present day Mars. This is likely the same case for the bassanite (localized bonded OH⁻). Geothite has no OH⁻ absorption feature and would be falsely noted as a non-hydrated mineral.

The remaining can be handled with additional evaluation of the overall shape of all the bands. The false positive H₂O at 1.93 μm in the analogue mineral spectra measured on Earth is most often a result of minor amounts of water being absorbed from the surrounding air. In the case of Earth analogue measurements, these false positives are considered a measurement artefact and is discounted in all cases but Halloysite, which has such a strong absorption feature that it

cannot be discounted. On Mars, there shouldn't be this type of error; however, if found in a pure mineral, it would be a potential indication for the presence of water in the mineral pore spaces.

There are several minerals that fall into the category of poly-hydrated minerals. These include coquimbite, epsomite, kieserite, and opal (spectra in Appendix C). In these cases, an "L" shaped curve is produced across the 5 channels and this can be used to identify the presence of water and water ice and/or a poly-hydrated mineral.

Four samples have the issue that the OH⁻ band has shifted from 1.4 μm out to 1.5 μm . In these cases, visual inspection of the shape of the 5 channels can indicate that they are likely hydrated with bonded OH⁻. This is the same with montmorillonite for the 1.93 μm water band. Olivine has a minor concave feature at 1.4 μm indicating the potential presence of OH⁻; however, evaluating the shape of the five bands shows a shape distinctive of olivine, demonstrating that it may be possible that olivine can be directly identified from the channel data. This is a similar method that is being utilized for the ExoMars Pancam for the detection and identification of minerals in the VIS-NIR frequency range (Cousins et al., 2010).

Analogue material measurement errors

The models of this thesis rely on accurate spectral measurement of analogue materials to determine the spectral shape, absorption features, and the correct reflectance values. IR spectroscopy was the method for measurement of the spectral characteristics of the different analogue materials. Data were gathered from a variety of sources, but results can vary, adding error into the model from the spectral measurements. Forms of error which can shift peak absorption features and intensity values include the sample preparation methods, variations in measurement methods (including the specific method and the equipment used for the measurement), and different mineral compositions despite having the same name. The measured intensities are especially important in order to discriminate variations in concentrations.

Sample preparation variations

The specific sample preparation protocol can lead to changes in the intensities of the absorption peaks for the measured spectra. The size fraction of the measured powder, clumping

of mixed minerals leading to a non-uniform distribution, particle orientation, and packing and levelling of the sample to be measured are the largest contributors to sample preparation attributed spectral errors. These were carefully controlled as described in Sections 2.3 and 4.4

The total variation (results not presented) was 4.4% for the basalt/gypsum mixture of 67/33 (see Figure 4-13).

Measurement methods and equipment variations

The collection and measurement of enough materials necessary for the models was beyond the scope of this thesis. The counter was to use material spectra from established databases; however, the results of any measurement can vary significantly, especially in terms of the measured intensity. In order to overcome this limitation, a method was developed to calibrate the scale to 0-1 diffuse reflectance and then adjust it to the maximum peak intensity of a series (Section 4.5). This shifted the measured spectra to a common point that allowed the comparison across different measurement methods and equipment. The error associated with this is due to the measurement error of the spectrometer and the KBr calibration standard. The spectral measurement error from the spectrometer was $\sim 4 \text{ cm}^{-1}$ (the resolution used during measurement), equivalent to 0.05 to 0.08% error for the 5 reflectance channels.

Material composition variations

The collection and characterization of materials is expensive and time consuming. The determination of optical constants is a huge task that is beyond the scope of this thesis. There are obvious advantages to leveraging data collected by other researchers; however, one of the biggest difficulties in comparing spectra across the different database to those collected for use in this thesis is that the materials composition can vary significantly. This will have a direct impact on the absorption peak positions and the measured intensities. The USGS samples were used as the preferred spectra as each sample was well characterized. This helped to ensure that the minerals were correctly identified. These spectra were matched to the collected samples to ensure a good match for laboratory testing. Some of the collected samples returned a spectrum that was markedly different from the database spectra, such as the montmorillonite sample. This sample was purchased from Wards but appears not to be pure montmorillonite when it was matched to

the Hapke generated spectra from the optical constants, and as such was eliminated from testing. The source was from a mine along a riverbed, and additional unknown sediments are expected to have been in the samples.

Likewise, optical constants were obtained from either literature or established researchers who have well characterized samples (Roush, 2005, Roush et al., 2007). Availability of optical constants is severely limited as these are difficult to measure.

To overcome these limitations, optical constants were matched to the measured spectra from the samples used in the models in Chapter 4 and 5 to ensure the correct spectral features and intensity (Section 4.5). For a couple of samples, the best case matching was used to determine which optical constant and powder fraction to use in the models. This was especially the case for the Basalt sample that was collected and sent for mineral characterization. While it was determined to be a high-CA pyroxene, it was not the same sample or composition that was used for the original optical constant measurements, and differences in the results were expected. Comparison of the measured pure spectra to the spectra generated from the Hapke model suggested that it was probably a weathered Palagonite (Figure 4-18); however, this was later considered incorrect as the best case matching for the channel ratios in Figures 4-53 and 4-54 suggested that this was, indeed, a pyroxene.

This confirms that good characterization of analogue data is critical to the development of the models, as well as surface or borehole cuttings data.

Radiometric model errors

The radiometric model errors are attributed to the design of the instrument and the component performance. These include manufacturers and measured data for the detectors, detector thermal stability, calibration target design and spectral response, additional sources of reflected energy within and beyond the field of view of the detector, detector window transmission errors, and LED thermal stability.

Manufacturers' detector data vs. Oxford measured data and thermal stability

The thermopile generates a voltage dependent upon the difference between the temperature of the detector and the scene temperature. This voltage varies directly with either of

these. When the temperature of the detector varies, this is counted as error, so keeping the temperature of the detector as stable as possible reduces the total error attributed to thermal variation. The detector thermal stability is the basis of the majority of the detector performance characteristics.

The performance parameters estimated for the thermal channels indicate that the instrument should function as expected to meet the performance specifications previously listed in Table 3-8; however, these are dependent upon a mix of manufacturers' data and measured performance of the detector in Oxford. The manufacturers' data was taken with a temperature set-point of the detector at 23°C, but there was no indication of the temperature variability in the test set-up. The application notes offered by the manufacturer suggest that it was in an open air space with thermal control of the air, rather than temperature control of the detector. In the testing of the detector as an individual component at Oxford, there was no thermal control on the detector in the clean room, relying on a mechanical chopper to eliminate the thermal background noise, instead. The instrument performance as designed is directly dependent upon thermal stability of the detector and its set-point. A different set-point yields a different voltage output for the same scene temperature (related to the temperature dependent off-set), while the thermal stability drives the D^* and SNR. The models in Chapters 4 and 5 utilized measured data from Oxford whenever possible, and then data from the manufacturers' datasheets as needed. Because of the differences in the testing methods, this assumption has unknown errors that could have the result of significantly decreasing the expected performance of the integrated instrument.

In the integrated instrument, thermal control of the detector will be required in order to reduce the error attributed to detector thermal stability. This is recommended here to be $\pm 1\text{K}$ as a starting point to testing. This will be updated in Chapter 6.

Estimated calibration curve assuming Spectralon and a Nextel painted target.

The normalization of values to a reference intensity will be done with a two-point calibration scheme with a Spectralon target as the reference to 100% diffuse reflectance and a Nextel painted target with an expected reflectance of near zero.

The Spectralon target as used in this study has an actual diffuse reflectance of about 98% across the spectral range of 1 – 2.5 μm . The manufacturers' spectra were used in the actual calculations for the models developed in Chapter 4 and 5 to account for this; however, this is for a pristine surface. The reflectance quality will degrade over time due to accumulation of surface dust and the breakdown of the compressed halon. It is important to keep the surface as clean as possible.

The high emissivity data point was measured with a Nextel painted aluminium target. In theory, a perfect black body target will have an emissivity of 1. In practice, creating a perfect blackbody simulator is quite difficult and any actual device will have an emissivity lower than 1. The flat target used in this study had a measured reflectance of 5-11%. Combined with a known temperature, it results in a good grey-body target that aids the calibration of temperature measurements as well as a reflectance calibration point. Similar to the Spectralon target, the quality will degrade over time due to accumulation of surface dust. It is important to keep the surface as clean as possible and to repaint as needed. If the surface is well characterized, regardless of condition, then the error will be based on the limitations of the measurement of the spectrometer.

Additional sources of reflected energy

If the emissivity of the scene is assumed to be 1, then there is no reflection term and there will be no associated reflected down welling radiance from outside of the scene. In practice, this is not the case and the energy emitted from materials surrounding the detector will be reflected and will have to be taken into account. Additionally, the detector will generate voltage for any object in the field of view that is at a different temperature, including the instrument components such as the sensor case, windows and filters, and probe casing. If these are at the same temperature as the detector, zero voltage is generated; however, in practice, there will be a temperature gradient across these components that will result in an unknown voltage component. Thermal control will be required to try to keep all of these components as close as possible to the same temperature as the detector in order to reduce this error. Calibration with the grey-body will help to reduce and characterize this form of error. The accuracy of this calibration and error will be

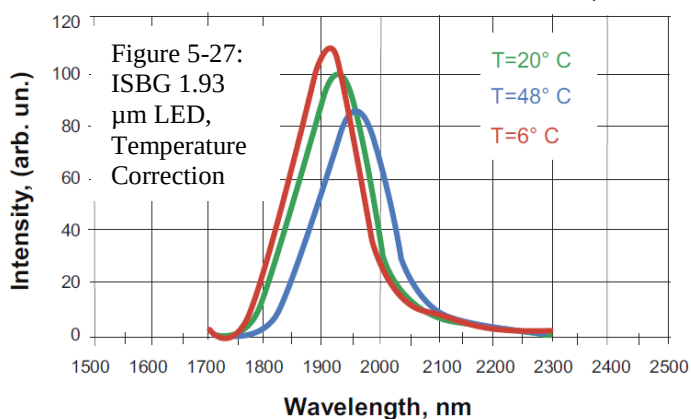
determined during the integrated instrument development and testing in Chapter 6; however, it is recommended to keep the thermal gradient across these to $< \pm 1$ K to match the thermal control of the instrument and LEDs.

Detector window transmission errors

The window transmission characteristics for the KRS-5 were taken from the manufacturers' data sheet (Figure 3-4). This is an ideal transmission curve. In practice, there are variations in the manufacturing process that will cause the actual transmission characteristics to vary. During the development of this thesis, one of the Dexter S25 detectors with the KRS-5 windows was destroyed. The window was carefully removed. An attempt was made to measure the window characteristics, but the windows were too small to be measured correctly by instrumentation in the laboratory. A shape of the transmission was obtained which represents the transmission characteristics, but the transmission percentage was not correct (data not presented). Rough scaling to the transmission value from the manufacturers data of $\sim 72\%$ indicated that there was about a 3% lower integrated transmission curve from 10,000 to 200 cm^{-1} when compared to the manufacturers' ideal curve. Since this is uniform across the channels, the same amount of energy is removed and the resulting absorption peak positions will remain the same, as will the ratio analyses.

LED thermal stability

The peak frequency emitted by the LEDs is also temperature dependent, as shown in Figure 5-27. This is the from the data sheet for the ISBG 1.95 μm LED. The peak frequency drops by about $0.045\text{ }\mu\text{m}$ as the operational temperature rises from 279 K to 292 K. Assuming that the integrated instrument will provide stable thermal control of the LEDs with the detector, this will be calibrated out with the Spectralon calibration target, as long as all measurements are made with the same LED temperature. There will be a difference in the model that can't



be calibrated out and an understanding of the temperature dependent energy emission variation of the LEDs is required to ensure that the *in situ* data can be interpreted from model data. The different LEDs will all vary with the temperature set-point, but this variation is design dependent. It is expected that each LED will require a different temperature set-point specifically designed to optimize both the peak emission frequency and the emission intensity; however, since the 1.95 μm LED has been shown to have the lowest SNR, these parameters should be designed for this LED. In this case, the temperature set-point for the LEDs, if not all independent, should be $290 \text{ K} \pm 1 \text{ K}$.

5.8 Additional local and regional data to assist in data interpretation

A final consideration in the Error analysis is that the data from this instrument will not be the only data available for the evaluation of sub-surface minerals. There are additional sources of information that will be available before the arrival to any destination on Mars and during the actual operations.

Remote sensing satellite data sets

Each landing location is carefully studied using all of the available assets around Mars prior to final selection as a landing site. This means that surface mineralogy will be understood and, in some cases, includes subsurface stratigraphy taken from local surface features. The existence of sub-surface water ice can also be determined from these assets. Cousins et al. (2010) suggested that bulk mineralogy from CRISM and OMEGA to aid in the design of Pancam filter sets and interpretation of data.

Remote sensing ground based data sets

This instrument will not be the only instrument on-board a rover or lander looking at the mineralogy. Pancam on ExoMars is a good example of another instrument which is determining the local surface mineralogy in real-time (Cousins et al., 2010). In all instances, this data would be utilized to determine a good spot to stop and drill prior to drilling, so assumptions on the expected types of minerals can be made. The range of minerals would be bounded and positive identification of the mineral with this instrument from the hydration state alone could be possible.

Drilling data

All the drills will have additional sensors on them to monitor the state of the drilling operations. This will provide information on the density of the subsurface environment that can help to identify mineral transition points and the presence of water ice. The combination of the surface instrument data with sub-surface allows the validation and interpretation of data in both directions.

5.9 Summary and expected performance of the integrated system

Thermal Channels

The theoretical performance of the thermal channel was demonstrated to meet the performance requirements of Table 3-8; however, some assumptions were made from the component performance data. Additional components that will affect the overall integrated system performance include the calibration of the detector to adjust for drift over time and the thermal stability. Some additional operational requirements were identified in this chapter, namely the performance requirements for thermal stability of the detector and LEDs. Each of these will be fully evaluated during the integrated system development and testing in Chapter 6.

Reflectance Channels

The results for the integrated power calculations compared to the Hapke model generated spectral results demonstrated that the functional system should be able to accurately measure the reflectance of the minerals in each channel. This included the capability to detect and discriminate water ice in a non-hydrated mineral matrix. It was also shown that both the 1.4 and 1.93 absorption features associated with the worst-case mixture of the hydrated mineral montmorillonite mixed with palagonite should be detectable in concentrations at least greater than 25% montmorillonite. It appears that the capability to discriminate finer mixtures could be difficult if the integrated system performance is lower than these calculations. It was also noted that more information from surface materials and borehole cuttings could improve models and interpretation of borehole measurements.

The SNR of 1.93 μm channel appears to be sufficient to meet the needs of this instrument, despite the tight range calculated for the palagonite/montmorillonite mixtures; however, the previous testing of the individual component performance (Chapter 3) combined with manufacturers' data in the expected instrument configuration demonstrated that it is at the threshold. The final instrument configuration and performance will have to be tested to ensure this can be achieved. Two key pieces of data are assumed which are the LED forward optical power data and the NEP. The 1.93 μm LED forward optical power appears to be the limiting factor. If the LED forward optical power is significantly lower than the data sheets and/or if the D^* of the integrated instrument is significantly lower than the measured data, the 1.93 μm channel could suffer significantly in performance. This suggests that an alternative detector (different manufacturer), instrument design, or channel combination that avoids the 1.93 μm channel should be considered whenever possible.

An investigation of an alternative to the 1.25-1.93 difference was performed for the 1.4 – 2.05 difference (Figure 5-21, 5-22, and 5-26). This is because the 1.4 μm and 2.05 μm LEDs are the two highest performing LEDs of the 5 with SNRs of 3.6×10^6 and 1×10^6 , respectively, for 100% reflectance. This would increase the energy reaching the detector by at least 1000x over the use of the 1.93 μm LED ratios. There would be some degradation in performance for this change. As noted in Figure 5-21 and 5-22, the 1.4-2.05 difference would limit the total range to 50% water ice content. In Figure 5-26, it is actually worse than the existing relationship. Because both the 1.4 and 2.05 μm bands are static with little variation with changes in concentrations of montmorillonite, the difference results are flat across the 0-25% concentration range, making this ratio useless for this combination of materials.

Instrument Performance Requirements Revisited

The requirements in the traceability matrix, Table 3-8, remain as they are with no updates from this chapter. Open data in Table 3-8 depends on the performance testing of an integrated prototype. Final specification values will be derived from that testing, and Table 3-8 will be updated accordingly.

Chapter 6: Bench-top Prototypes and Testing

6.1 Abstract

The objective of this chapter was to develop, build, and test integrated technology demonstration units for the thermal and reflectance channels. These units included the components that were selected and tested in Chapter 3 and were tested with materials that were identified in Chapter 2. The purpose of these demonstration units was to validate the integrated system models that were developed in Chapter 5.

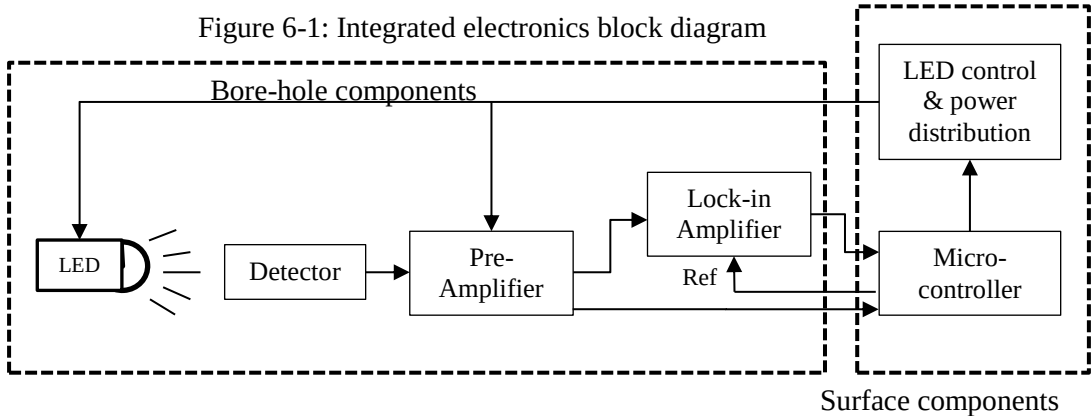
The thermal and reflectance channels were developed and tested separately with several iterations in the experimental design and hardware. These were tested on the bench-top and in a simulated environment, when appropriate. This approach to the development of the project provided: 1) the necessary confidence that the selected technology solution will perform as predicted, 2) development of specific testing methodology and protocols, and, 3) confirmation of the integrated system performance requirements. An integrated technology demonstration unit was built from the recommendations of the individual thermal and reflectance channel testing.

This chapter presents the results of all testing and the detailed design of the integrated technology demonstration unit including the optics, mechanical, electronics, and software components. It concludes with an update to the final performance specifications for a future flight instrument design.

6.2 Integrated electronics and preliminary pre-amplification circuit

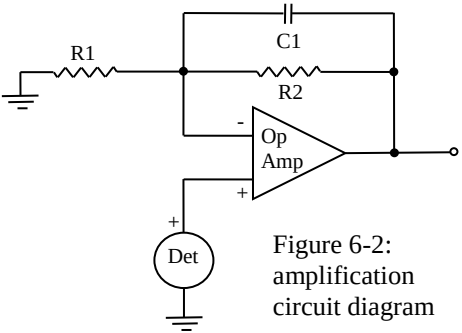
The majority of the integrated electronics will be presented in the integrated technology demonstration unit section (6.7); however, the detector output pre-amplifier is an important component that was developed early in order to minimize signal noise. The block diagram (Figure 6-1) shows four major components to the electronics and power distribution system. This includes: detector output signal pre-amplifier, a lock-in amplifier, LED control and power distribution board, and the microcontroller. An external computer and power supply are in

addition to these components. The pre-amplifier and lock-in amplifier are the central subsystems to the electronics that have a direct impact on the performance of the integrated instrument. The purpose of the pre-amp component is to boost the detector signal over other sources of noise such as thermal, electrical, or from the other components. It needs to be close to



the detector output to minimize noise.

The settings of the SRS Pre-amp and Lock-in amp during the D* testing in Chapter 3 were used to design an amplification circuit necessary for the integrated instrument. A recommended amplification circuit (Figure 6-2) by the thermopile



manufacturer, Dexter, was modified after the results of the D* testing (Chapter 3).

A base design was built and tested for early channel prototype development. The rest of the electronics and the final detector output signal pre-amplifier will be presented in the integrated prototype section (Section 6.7). The minimum amplification requirement was set to 1000x (per detector testing presented in Chapter 3), and resistor and capacitor values were selected to

Table 6-1: Specifications for Amplifier Circuit			
Item	Value	Selected Component	Component specification
Op Amp	-	Analog Devices AD470	Very low noise
R1	75 Ω	Panasonic ERA3A-0603 Farnell P/N: 1670161RL	100mW, $\pm 0.1\%$, ± 25 ppm/C $^\circ$
R2	75 K Ω	Panasonic ERA6A-0805 Farnell P/N: 1717675	125mW, $\pm 0.1\%$, ± 10 ppm/C $^\circ$
C1	0.01 μ F	AVX – 06035C103K4T2A	CAP, MLCC, X7R, 10NF, 50V, 0603

optimize the amplification and reduce feedback noise (Table 6-1).

The results of the testing determined that the circuit amplification was 999.58x. An estimated error of about 0.07% was attributable to the amplification circuit.

This configuration provided a basic set-up that could be used for bench-top testing of the thermal and reflectance channels. The integrated field instrument will require a PCB with surface mount components in order to reduce the noise attributed to the electronics. Surface mounted components have the advantage of using less solder and bonding materials, and this reduces the resistance and noise. Thermal stability is an important issue, so this design and analysis will be revisited in integrated instrument design and testing.

6.3 IR Thermal Emission Measurement: Channels A & B

The selection of the two thermal bands was discussed in section 2.5. These are a narrowband (Channel A) and a wideband (Channel B).

The principle components for the instrument in these channels included the detector, amplifier, and filters (Table 3-6). In order to control temperature variations in the detector, the design required an iso-thermal block (aluminium), thermocouple temperature sensors, a heating element, and a temperature control system. Additionally, external data-logging of temperatures and detector voltages was necessary. The experimental design was designed to limit reflected energy from reaching the detector from sources other than the scene.

The bench-top development of the thermal channels included the design and testing of two prototypes. The first prototype (Thermal Prototype I) tested the basic concept (instrumentation and testing methods) while the second prototype (Thermal Prototype II) was developed in the form of a borehole instrument with improvements to the experimental design to simulate a borehole environment.

Thermal Prototype I

The purpose of the Thermal Prototype I was to test the three main components (detector, filter, and amplifier) across a simulated scene temperature range of 175 K to 310 K. The

experimental design was developed to provide both independent thermal control and thermal isolation of the detector and scene. Data were collected to determine the system performance in order to make recommendations on thermal control and experimental design for an improved, borehole configuration prototype.

Methods

Configuration

The experiment was set up and run in a thermal vacuum chamber (Figure 2-2). Figure 6-3 shows the experimental setup within the vacuum chamber. The Dexter S25 thermopile (Fig. 6-3, item 'A') was mounted in a support bracket ('B') over a grey-body target ('G') so that the detector would only see the target in the scene and nothing else.

The Dexter S25 Thermopile has a KRS-5 window. This was used as is for the broadband Channel B. A second 25.2 μm filter was placed in front of the detector window for the narrowband Channel A. This was secured to the aluminium support bracket with Kapton tape, and was the extent of the thermal connection between the filter and the detector.

Thermal control

A type N thermal grease made by Apiezon (for low temperature thermal vacuum operations) and a bracket were used to thermally couple the detector to the sensor support bracket. A heater and a thermocouple were also thermally coupled to the sensor bracket.

It was assumed that the temperature of the thermocouple on the sensor support bracket represented the actual temperature of the detector for the purposes of the calculations, though some thermal lag between the two was anticipated. Thermal stabilization of the sensor was accomplished by monitoring the temperature and manually varying the voltage to the heater. A set point of $294.4\text{ K} \pm 1\text{ K}$ was selected and maintained for these experiments.

The PTFE sensor support post ('F') broke the thermal connection between the cold plate base and the sensor support bracket, so that any heating/cooling was associated only with radiation from the grey-body.

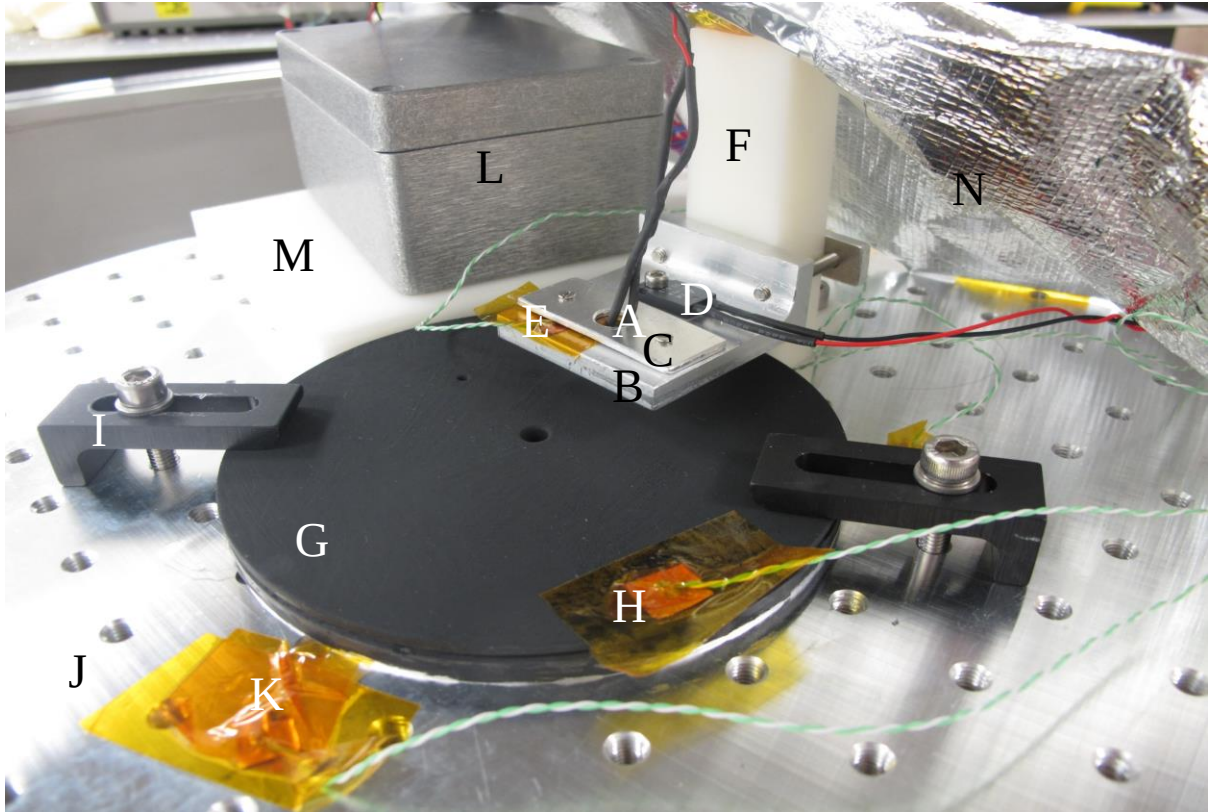


Figure 6-3: Experimental Setup for Testing of Thermal Prototype I

- | | |
|--------------------------------|--------------------------------------|
| A) Dexter S25 Thermopile | H) Grey-Body Thermocouple (x2) |
| B) Sensor Support Bracket | I) Bolts |
| C) Sensor Clamp Bracket | J) Cold Plate Base |
| D) Thermal Heater | K) Cold Plate Base Thermocouple (x2) |
| E) Sensor Thermocouple | L) Amplification Electronics |
| F) Sensor Support Bracket Post | M) Thermal Separator |
| G) Grey-Body | N) Mylar Blanket |

An MLI blanket ('N') was placed over the experiment in order to thermally separate it from the vacuum chamber walls. This broke the thermal connection with the vacuum chamber walls so that there was no heating/cooling link between the experiment and chamber walls.

"Grey-body" calibration target

A true "Blackbody" has an emissivity = 1. The calibration target was designed to have as high an emissivity as possible, but the emissivity was < 1 , so it is really a "Grey-body" (e.g., a surface with known emissivity and temperature). The grey-body was prepared in the mechanical shop by lathing off the top and bottom so that they would be parallel. The top surface was sandblasted and then painted with Nextel black paint (3 coats of primer followed by 3 coats of

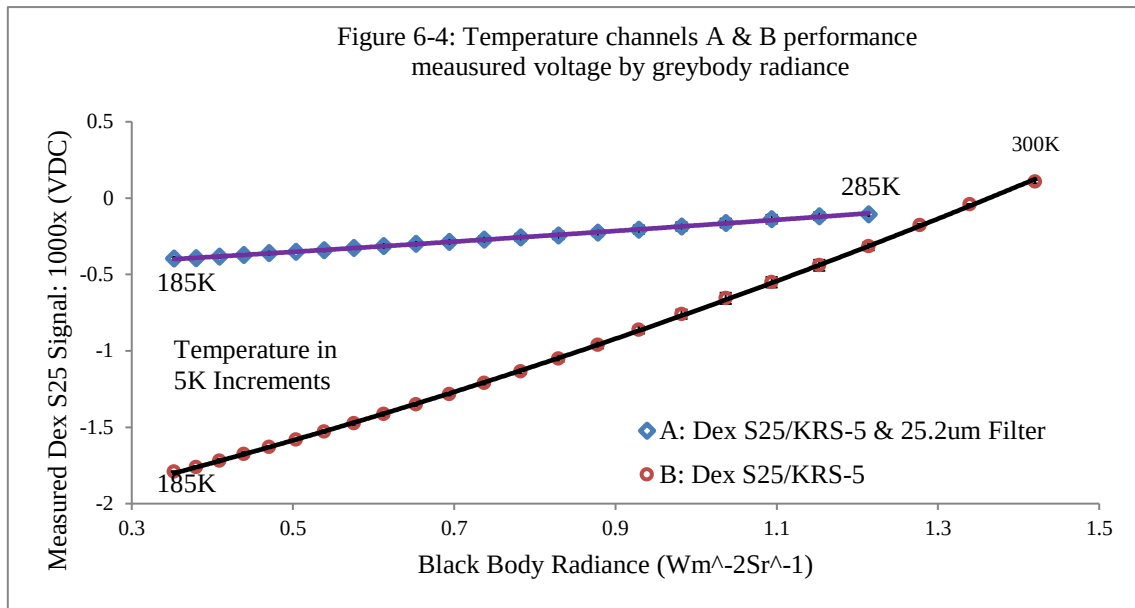
the paint). The emissivity is dependent upon the preparation of the painted surfaces and number of coats. The Nextel emissivity was assumed as 0.95 at $\sim 25\text{ }\mu\text{m}$ (Channel A Centre Wave Length), per the manufacturers' specification. The bottom of the grey-body was left natural with no painting or other treatment. A thin coating of type N thermal grease was applied just before it was bolted to the Cold Plate Base ('J'). This thermally coupled the grey-body to the cold plate base. Temperature was measured with a type K thermocouple that was added to the bottom side of the grey-body with double-sided tape and covered with aluminized Kapton to ensure it was thermally coupled to the grey-body. It was then covered with a Mylar Multi-Layer Insulation (MLI) blanket to separate it thermally from the cold plate base. A second type K thermocouple was placed on the top side of the grey-body. This allowed a reasonable measurement of the actual scene temperature that was used for the calculations.

Experiment protocol

The chamber was evacuated to about 6.9×10^{-6} bar and the temperature of the vacuum chamber instrument bench was varied from $\sim 175\text{ K}$ to $\sim 310\text{ K}$ in four cycles ($n=4$) via the cold head.

Results

Channels A and B were tested in separate experiments with the same conditions. The results of testing the temperature channels A (Dexter S25 w/KRS-5 window with $25.2\text{ }\mu\text{m}$ filter) and B (Dexter S25 w/KRS-5 window) are presented in Figure 6-4. Four cycles for each configuration were averaged and the standard deviation calculated. The bottom and top temperature in the data run are indicated next to the associated data point with 5 k increments from top to bottom. The integrated channel radiance was calculated per equation 4-1, for each temperature. This was plotted against the measured voltage through the temperature range, interpolated to whole number increments.



Discussion

The results (Figure 6-4) show that the detector response is stable and repeatable. Channel B had more dynamic range (because of the larger amount of energy reaching the detector) as compared to Channel A with the additional 25.2 μm filter. The best fit for both channels was a 2nd order polynomial fit. Channel B has a larger polynomial component, resulting in a more visible bend to the fit. When plotting the voltage against the black body radiance, a linear fit is expected, and a polynomial fit is due to several error and deficiencies in this experimental design and testing.

The first is that the manual thermal control of the heater was not sufficient, resulting in significant thermal variation. Variations in the detector temperature have a direct effect on the signal voltage that is measuring the temperature difference between the detector and the scene temperature. This means that the integrated instrument will be required to have active thermal control of the detector. The detector should also be mounted in a thermal block such as aluminium or Al/Cu. The specific temperature stability requirement will be driven by the performance of channel A with the narrow band 25.2 μm filter. Because much less radiation reaches the detector, thermal variability will have a more pronounced effect on the output signal and error for the narrowband (Channel A), than with just the KRS-5 wide band window (Channel B). A detailed analysis is required to determine the point in which the emissivity cannot be determined due to the variation in temperature; however, from visual inspection of these results, it is anticipated that thermal stability will need to be about 100 mK (0.1 K). A secondary problem was that the up/down

thermal cycling approach didn't allow the greybody to stabilize at a temperature for long enough so that the total number of data points averaged for a temperature were too few, increasing the error. A change to the experiment thermal cycling scheme will be required for the next thermal prototype.

The second major issue is related to an un-accounted reflectance term in the radiance calculation. In this test, it was assumed that all the energy reaching the detector was emitted from the greybody source. As was explained in section 5.7, in the subsections, *Estimated calibration curve assuming Spectralon and a Nextel painted target* (page 5-28) and *Additional sources of reflected energy* (page 5-29), the grey-body Nextel target has a reflectance term on the order of about 5%. This allowed energy from beyond the scene to be reflected into the detector. Additional sources included the Mylar blanket over the experiment, the brackets, and cold plates. The integrated instrument model results in Figures 5-7 and 5-8 also assumed that there would be no reflected energy beyond the scene. This will have to be accounted for in the next thermal prototype and experiment design.

Another portion of the un-accounted radiance term was attributed to components within the scene that were at a different temperature than the detector. This included the windows, filters, and any other part of the instrument that were in the field of view of the detector. The best approach to solving this problem of un-accounted radiance terms is to design to eliminate these sources entirely from the field of view of the detector. Another approach is to thermally couple these components to the instrument and maintain them at the same temperature as the detector in order to eliminate these additional radiance sources. The final option is the measurement of their temperatures in order to account for these in the calculations. The final solution will probably have to utilize all of these options.

The 25.2 μm filter in channel A is the most challenging to thermally couple. The only location to do this is along the edges. This filter has the most direct exposure to the viewing scene and is the primary thermal heat path. The centre of the filter will have to be free of obstructions, and this design results in a thermal gradient from the edge to the centre of the filter. In a flight instrument, the filter material will be known and can be thermally modelled based on the final

design to account for a gradient and a radiance term associated with the filter. For this device; however, a custom fabricated filter was not within the project budget. The performance of the wideband channel B has been shown to be reliable in Figures 5-8 and 6-4. The calculations for Channel B with Mini-TES bulk, undisturbed surface spectra (Figure 4-3) indicated that the error from the emissivity in the wideband channel would be $3.19 \pm 0.77\%$. Because the performance was expected to be sufficient for testing with the wideband, and because of costs, it was recommended that the next thermal prototype proceed with just the wideband channel B.

Another key issue was that there wasn't sufficient thermal separation from the vacuum chamber walls and Mylar blanket over the experiment. This allowed heat from the room environmental control system external to the experiment to translate all the way through to the detector. This was a significant portion of the additional reflected radiation that was not accounted for in the blackbody radiance calculation. An upgrade to the thermal isolation design was recommended for the next thermal prototype.

There are additional minor sources of error. One is the signal noise from the amplification circuit. Because the circuit is set away from the detector, noise is created along the wiring between them from resistance and line temperature variations. The other minor source of error is from the transmission characteristics of the actual KRS-5 window in the sensor that may not strictly match the manufacturers provided data. Transmission characteristics were obtained from the manufacturers' website from a general diagram of all of their windows; however, there are no data for the actual performance of what was shipped. An attempt was made to measure the transmission characteristics, but not fully successful. An estimated error is $< 0.5\%$.

Conclusions and Recommendations for Prototype II

Channels A and B have been shown to be fully functional and will allow the measurement of the required temperature range. Channel A would allow the measurement of the brightness temperature as the $25.2 \mu\text{m}$ narrow band range was selected to optimize the emissivity of a variety of samples to be as close to 1 as possible.

A number of recommendations for the next thermal prototype included the following:

- Test the device in the correct dimensions and form of a borehole device.
- Simplify the design to test just the wideband configuration to reduce the design complications of having a second filter in front of the detector that would not be fully thermally coupled to the detector.
- Provide digital control of the thermal stability of the borehole device.
- Keep the wiring as short as possible between the detector and amplifier.
- Create a borehole simulator surrounding the instrument and scene that is thermally coupled to the cold-head so that all radiation sources are at the same temperature as the scene.
- Add more Mylar (MLI) to provide further thermal separation of the experiment from the vacuum chamber wall.
- Modify the experiment temperature cycling to allow more time to stabilize at each temperature.
- Create a model of the integrated system to determine the performance of the actual system compared to the theoretical performance.
- Test against physical analogue samples.

These recommendations provided the basis for the development and testing of the Thermal Prototype II.

6.4 Thermal Prototype II

The results and recommendations from Section 6.3 were used to design and test a second prototype and experiment design for a borehole instrument configuration. External equipment provided thermal control, data-logging, and power. This allowed testing of the instrument in order to determine the performance requirements for an integrated instrument.

This set of testing included the blackbody target and the physical samples of Morocco basalt and CaCO_3 as described Table 2-4. The results of these were compared to a theoretical prediction of the radiance expected for this instrument and experiment configuration against these samples.

Thermal Prototype II Design

The thermal stability of the detector is a critical item in the development of the integrated instrument prototype. This required providing a thermal block that could be temperature

controlled and that was thermally isolated from outside sources. This was implemented with a three-layer design shown in the concept drawings in Figure 6-5. The bore diameter of 25 mm was used as the primary constraint in the design with the dimensions of the detector as the second. All layers were designed around these two constraints.

The as-built Thermal Prototype II is shown in Figure 6-6. The device included the detector, a low-power ceramic, resistive heater, and two thermocouples.

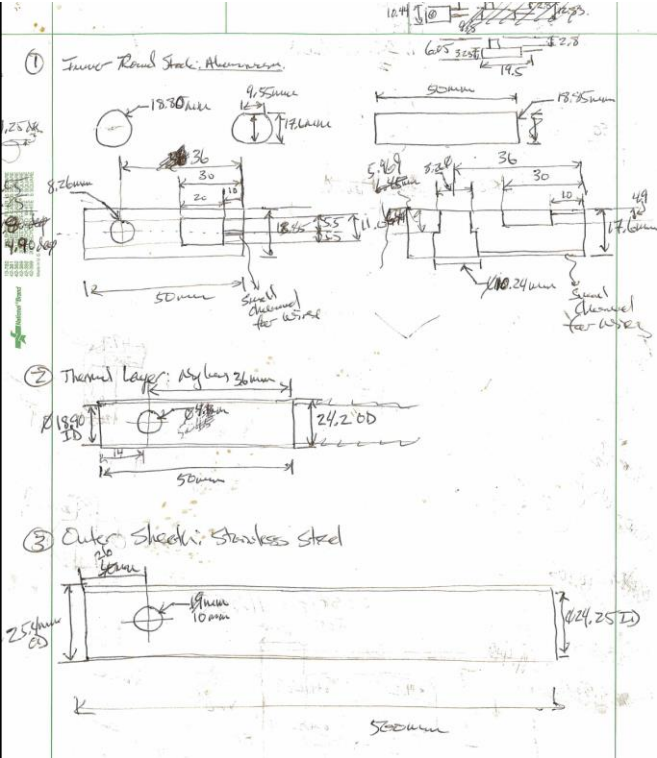


Figure 6-5: Thermal Prototype II Concept Drawings

The hole centred over the detector window was sized and placed to allow an unrestricted

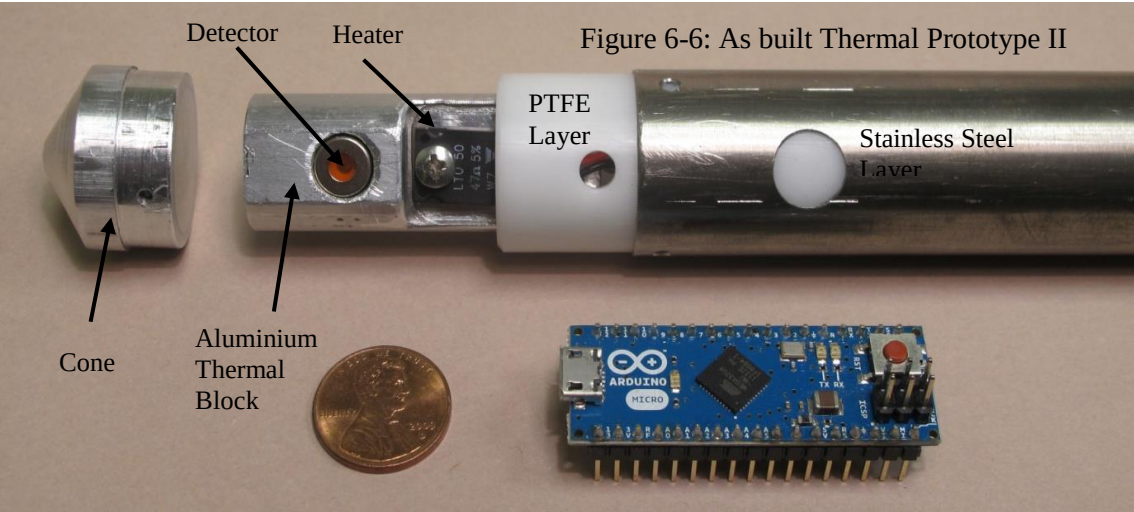


Figure 6-6: As built Thermal Prototype II

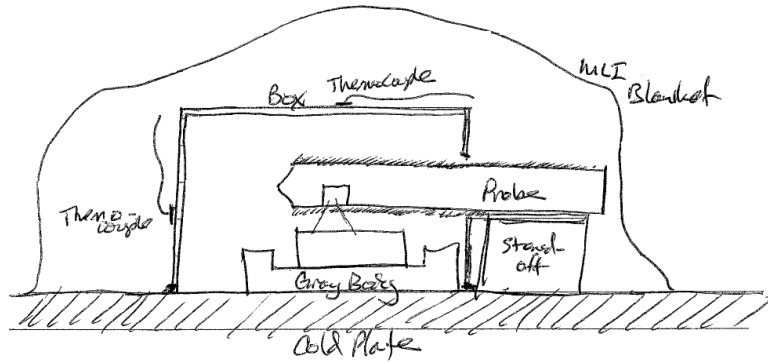
full Field Of View (FOV) of the detector to the scene. This was to ensure the highest flux would reach the detector.

Mars borehole simulator

The development of a Mars Borehole simulator was a key addition to this experiment. This was necessary to eliminate thermal emission radiance sources beyond the scene. A concept

of the solution is shown in Figure 6-7. A standard die-cast aluminium electrical box was modified with a hole for the probe. The edge was milled flat and thermally

Figure 6-7: borehole simulator design concept



coupled to the cold head plate with thermal grease and clamps so that the temperature of the box on all sides was close to the temperature of the greybody or sample. The inside surface was painted with Nextel in order to reduce the reflectance and to make an isothermal cavity. This helped to reduce the amount of thermal signal radiated from the environment through the vacuum chamber walls.

Experiment

Method

Testing of the TPII followed TPI testing (Section 6.3) with the following additions:

Configuration

The instrument (Figure 6-6) was covered in Mylar to reduce the amount of reflected radiation from the surfaces outside of the scene and then mounted over a greybody target using a block of PTFE to support it and thermally separated it from the cold plate (Figure 6-8). The target surface was clamped to the cold head

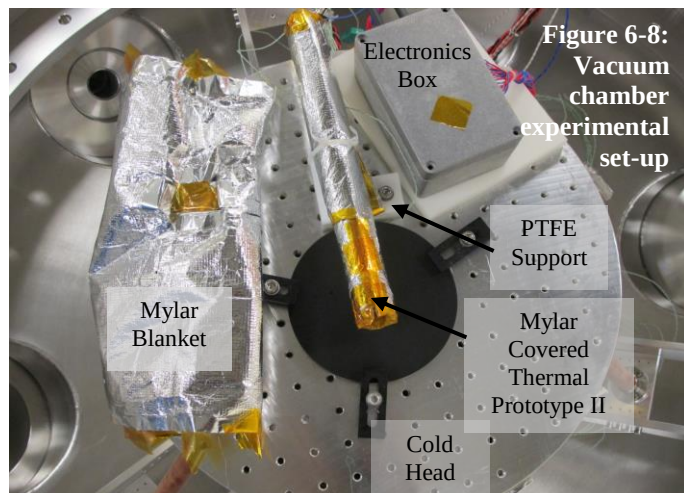


Figure 6-8: Vacuum chamber experimental set-up

plate, the borehole simulator box was set around the experiment and clamped top the cold head plate, and then the Thermal Probe II was placed through the hole over the target surface (Figure

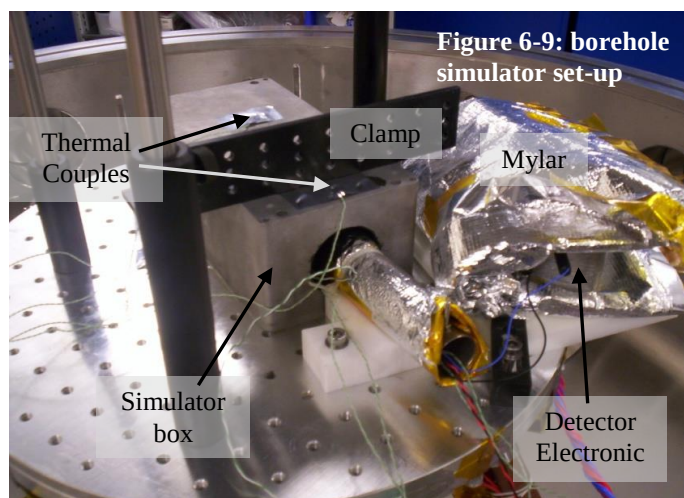


Figure 6-9: borehole simulator set-up

6-9). Thermocouples were attached to the side and top of the MBHS to record temperature data necessary for refining radiance calculations. An MLI blanket was placed over the entire experiment to further thermally de-couple it from the vacuum chamber walls. Thermal control of the instrument was accomplished with a Eurotherm 2116 proportional-integral-derivative (PID) controller, which controlled the voltage to the ceramic heater.

Protocol

In the Thermal Prototype I testing, part of the temperature variation was attributed to not having enough time to stabilize at each temperature. For the Thermal Prototype II experiments, the thermal cycling protocol was modified to a four-point calibration approach in which a Eurotherm 2116 used to control the vacuum chamber cold head temperature was programmed with a 4-step cycle. Each set-point would be allowed to stabilize for several hours.

The four set-points were 200 K, 220 K, 240 K, and 260 K. A short and long protocol were used in the experiments. The settings for the two versions of the thermal cycling protocol are provided in Table 6-2.

Table 6-2: Thermal Cycling Protocol

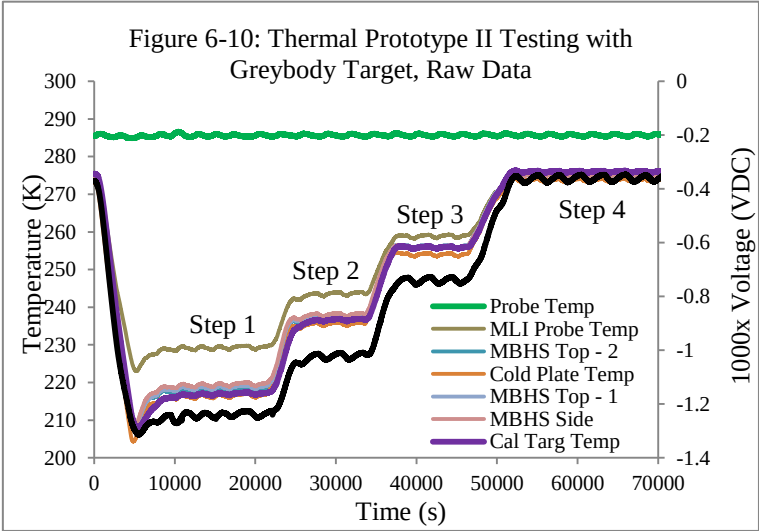
Step	Temp Set-point (K)	Hold Time (hrs)	
		Short	Long
1	200	3	5
2	220	2	3
3	240	2	3
4*	260	2	3

* Hold until manual shutdown

The probe had a temperature set-point of 285 K for the testing (which varied ± 1 K); however, data were only selected when the probe temperature was within a 285.7 ± 0.1 K (100 mK) range. Additionally, during calibration, a target scene temperature was selected for the blackbody target with an allowable variation of ± 0.1 K. Both criteria had to match in order for data to be selected. From 3-10 minutes of data were averaged for each temperature set-point.

Results

Figure 6-10 provides an example of the typical raw data collected for the



greybody target measurement. An example of the averaged data for each set-point is provided in Table 6-3 for the greybody target measurement. Radiances were plotted against the measured voltage in Figure 6-11, 6-12, and 6-13 for the greybody target, basalt, and CaCO_3 , respectively. The results for all three experiments are compared in Figure 6-14.

Table 6-3: Thermal Prototype II Testing with Greybody Target, Raw Data

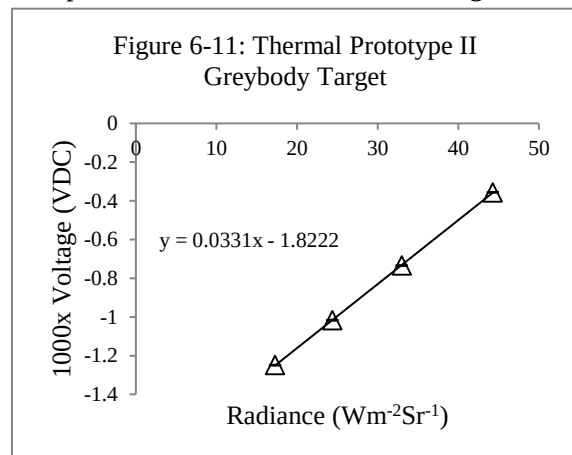
Cold Head:	200 K		220 K		240 K		260 K	
	Cal Targ Temp	Detector Voltage	Cal Targ Temp	Detector Voltage	Cal Targ Temp	Detector Voltage	Cal Targ Temp	Detector Voltage
Average:	216.720	-1.24936	236.782	-1.01722	256.047	-0.73464	276.144	-0.35637
Stdev:	0.0560	0.001887	0.0493	0.002294	0.0362	0.002186	0.0143	0.001665
% Error:	0.0026	-0.1511	0.0208	-0.2255	0.0141	-0.2976	0.0052	-0.4672

Experiment Results Discussion

Grey-body target testing

An example of the experimental raw data for the grey-body target is provided in Figure 6-10. The four-step protocol is clear. The thermal stability of the probe (dark green) oscillates around the set-point of 285.7 K with a variation of about 1 K. The thermal stability of the blackbody target (purple), or rock chips in subsequent tests (data not shown), oscillates around the set-point of the cold head (taking into consideration thermal lag across the physical boundaries) with a variation of ± 1 K. The detector voltage (black) tracked both the step changes and the temperature oscillations of the probe and target temps.

As can be seen in Table 6-3, there was about a 16 K difference between the cold head setting and the actual temperature of the target. Temperature variation of the actual target in the selected data range was below 56 mK while the detector voltage variation was around 2 mV. Radiances for each of the four temperatures were calculated for the experimental set-up per the model that was developed in Chapter 5. These were plotted



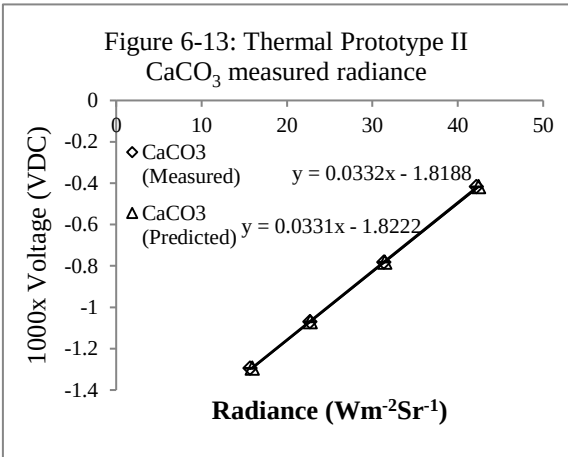
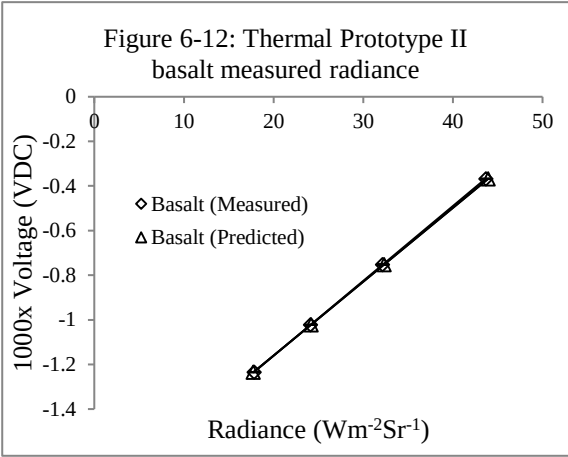
against the measured voltages for each temperature (Figure 6-11). Error bars are per the calculated voltage error in the Table 6-3 with a range of 0.2 to 0.5%. This was used as the calibration curve for fitting the basalt and CaCO_3 data.

Basalt

The measured results are compared to the predicted in Figure 6-12. The predicted radiances, given the same temperature points, were calculated using the calibration curve (see Figure 6-11) and closely matched the predicted radiances (Table 6-4). Error bars are per the calculated voltage error with a range of 0.2 to 0.4% (data not provided).

CaCO_3 Rock Chip

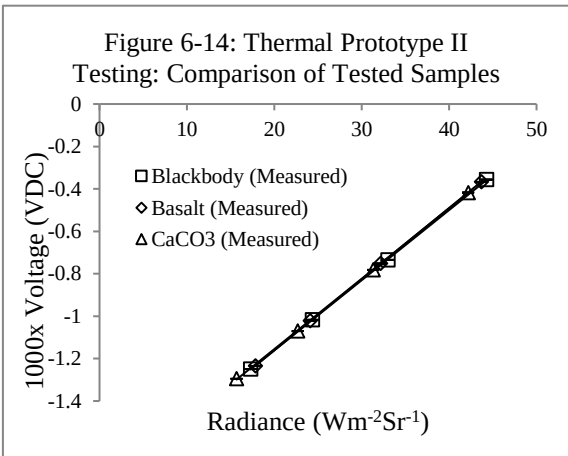
The CaCO_3 has an average emissivity of about 0.72 in the 1 to 30 μm range (average of data from Figure 2-8), so there was a reflectance term that needed to be added to the total radiance in order to match



the measured to the predicted voltage. This term was calculated from blackbody radiances for the average temperature of the box surrounding the probe and added to the radiance term calculated for the CaCO_3 temperature and plotted in Figure 6-13. Error bars are per the calculated voltage error with a range of 0.1 to 0.3%. The measured radiances closely matched the predicted radiances (Table 6-4).

Comparison of Measured Results

A comparison of the results for the three tests is presented in Figure 6-14. As expected, the results of the blackbody target



and basalt rock chip are quite similar while the CaCO_3 sample was significantly separated from the other two surfaces due to the lower emissivity term.

Temperature measurement performance calculations

A comparison of the temperature measured by the bench-top instrument verses the actual measured value was performed for the basalt and CaCO_3 rock chips tests. The actual measured temperature was plotted against the actual voltage measured. A second order polynomial was fit to the data resulting in an equation of the line (Figures 6-15 and 6-16). A look up table was generated for this equation with temperatures from 200 to 300 K with a 0.1 K resolution (as previously described in Section 1.9). This was used to generate a set of predicted voltages. The resulting temperature error for Basalt was 3 to 90 mK while the error for CaCO_3 was 50 to 210 mK (Table 6-4).

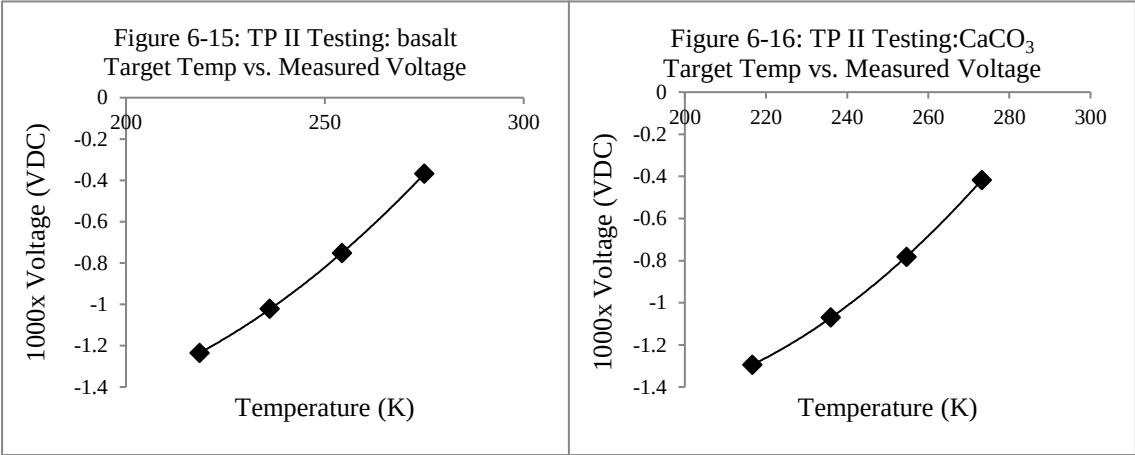


Table 6-4: Comparison of Thermal Prototype II measured to predicted with basalt and CaCO_3

Step	Basalt				CaCO_3			
	Voltage	Temperature		Diff. (K)	Voltage	Temperature		Diff. (K)
	Measured (VDC)	Measured (K)	Predicted (K)		Measured (VDC)	Measured (K)	Predicted (K)	
1	-1.23496 ± 0.000293	218.517 ± 0.041	218.44	0.07	-1.29516 ± 0.001071	216.600 ± 0.066	216.55	0.05
2	-1.0221 ± 0.003586	236.164 ± 0.066	236.25	0.09	-1.07024 ± 0.002104	235.933 ± 0.054	236.05	0.12
3	-0.75198 ± 0.002061	254.322 ± 0.049	254.25	0.07	-0.78187 ± 0.001403	254.629 ± 0.049	254.55	0.08
4	-0.36745 ± 0.001601	275.053 ± 0.033	275.05	NET	-0.41739 ± 0.001292	273.141 ± 0.039	273.35	0.21

System performance calculations

The performance of the system was calculated using similar methods for determination of the performance of the detectors at the component level. Data for the testing of the Thermal

Prototype II with the Blackbody target (Figure 6-10) was used in the calculations that used a two-point temperature calibration method as previously described in Figure 3-7.

The temperature range allowed for the analysis were ± 10 mK on the probe and ± 50 mK for the blackbody target. The results are provided in Table 6–5.

Table 6-5: Performance of Thermal Prototype II

Parameter	Value
NER ($\text{Wm}^{-2}\text{sr}^{-1}$)	0.0007
NEP ($\text{nW}/\text{Hz}^{1/2}$)	0.01
D^* ($\text{cmHz}^{1/2}\text{W}^{-1}$)	1.55×10^9
SNR	3.32×10^7

General Discussion

Thermal stability of the detector

Thermal stability is essential to the performance of this instrument, so this was carefully controlled in order to understand the thermal performance requirements for an integrated field instrument and to demonstrate the capability of the bench-top instrument to meet the science requirements (Table 1-4).

The temperature control of the probe in this design was dependent upon an external cold-sink combined with a Eurotherm PID controller. This was because there was only active heating (the ceramic heater) as opposed to active heating and cooling that might be accomplished with a Thermal Electric Unit (TEU) type solution. In this case, the cold plate served as the cold-sink. The geometry of the experiment and the separation of the probe from the surface determined how fast radiated heat could be transferred from one surface to the other, and barriers to heat transfer were created to reduce this thermal heat flow (e.g., PTFE stand-off and MLI blanket around the probe). For this design, testing of the system determined a temperature set-point that could be maintained at the coldest setting (Step 1) while keeping the voltage to the heater to the minimum amount to avoid over-powering the temperature control at the warmest setting (Step 4). This resulted in a temperature set-point for the probe of 285 K for the testing (which varied ± 1 K) and 6 VDC to the heater, while data were selected across all the final experiments for a probe temperature of 285.7 ± 0.1 K. The heater drew about 0.1 Amps, for an estimated power draw of 0.6 watts.

Thermal stability of the scene

In parallel to the heater control, the temperature of the calibration target and samples were controlled by thermally coupling them to the cold-plate with clamps. This provided the scene temperature for the experiment. The cold head was set to a temperature with a Eurotherm controller and allowed to stabilize over the course of several hours. The cold head temperature oscillated around the set-point at about ± 1 K. A scene temperature was selected for each step and a range of ± 0.1 K was allowed for data selection. In order for data used in the analyses to be valid, they had to fall within both ranges of scene temperature and probe temperatures. Because these were controlled independently, the oscillations did not necessarily align, so a lot of data were required to allow enough data points to be collected. Even with the ± 0.1 K range limitation, this was quite generous and allowed 3-10 minutes of valid data points to be collected at multiple oscillations during a step. The averaged data and resulting error was well within the original requirement set out in the science requirements traceability matrix of ± 3 K (Table 3-8). In these experiments, the performance ranged from 0.003 to 0.21 K difference between the measured and predicted temperatures (Table 6-4). For the most part, the predicted values fell within 2-sigma of the measured error. The largest errors were with the CaCO_3 . This is attributed the average emissivity of CaCO_3 of 0.72. The results of this test suggest that the integrated field instrument will require temperature stability of at least ± 0.1 K, or at least carefully controlling the calibration to select a smaller range of temperatures when selecting data. This is also a reasonable approach as long as it is consistent for both calibration and samples.

Forms of errors

The primary forms of error due to thermal control that were identified during the Thermal Prototype I testing were mostly overcome with the addition of digital PID control of the probe temperature and thermal isolation with the layered instrument design and the MLI external layers. The extensive thermal testing for the experiment protocol resulted in a thermal cycling protocol that allowed the target surface temperatures to stabilize. The measured results compared

favourably to the predicted results. The original assessment that thermal stability would need to be about 100 mK was demonstrated with the Thermal Prototype II design.

Secondary forms of error included potential added noise from the placement of the amplification circuit in relation to the detector. This was not clearly demonstrated in this testing, so it is likely any signal noise was over-powered by the thermal noise. This is the same for the KRS-5 window spectral response, which is not directly known.

Detector Performance

The results of the Thermal Prototype II testing met the performance requirements (Table 3-9). The device as designed was tested and demonstrated to have a 1 magnitude better performance for the NEP and for the D^* when compared to the manufacturers data (Table 6-5). This was because of the use of the full FOV and placement close to the samples, which maximized the flux reaching the detector. This was also due to thermal stability of the detector and scene under ideal operational conditions in the vacuum chamber set-up.

Wideband vs. Narrowband

The method for calculating the total radiance necessary to predict the expected temperature from the voltage reading is sensitive to the spectral response of the window on the detector. In this round of testing, the wideband version was selected in order to reduce the complexity of the testing; however, this meant that knowledge of the spectral properties of the environmental sample being measured were also necessary. This is demonstrated by the results of the basalt sample being similar to the greybody target, which have nearly the same emissivity (~ 0.95), while the CaCO_3 sample with an emissivity of about 0.72 had to have an additional reflectance term accounted for in the calculations (Chapter 5).

The point of the narrow-band filter is to select a band-pass where the emissivity across all the typical Mars minerals is as close to unity as possible (see Figure 2-9 as an example). A narrowband filter combined with good thermal stability would allow a device that is both accurate and can measure the surface temperature independent of knowledge of the spectral properties of the target sample material. However, the total radiation passing through the narrowband filter is significantly reduced (in comparison to the wideband window), and this will result in a decreased

signal to noise ratio. The results shown in Figure 5-7 indicate that this should not be an issue for the detector.

Recommendations for the Integrated Field Instrument

Specific recommendations for the integrated field instrument for the thermal channels are as follows:

- Follow the same layered concept with the probe design and thermally couple the detector in the inner aluminium block to reduce the thermal variability
- Design and build a PCB with the pre-amplification circuit miniaturized and mounted to the back of the detector can to shorten the electrical leads as much as possible. Similarly, place a copper layer in the PCB to shield the detector output signal leads
- Build a prototype with the correct geometry of a bore-hole instrument with the wideband channel to test performance with known samples
- Keep thermal control of the detector to be within ± 100 mK of a specified set-point, or at least limit valid data points to be within this range.

6.5 IR reflectance measurements to determine water ice and hydrated minerals

In the reflectance channels, voltage is generated from IR energy reflected off a surface. The reflected energy detected is dependent upon the surface spectral characteristics, the IR source, and any windows or filters in-between the source and the detector. Filters and LEDs were previously selected and tested in sections 3.4 and 3.5, respectively. See Table 3-7 for the full listing by channel.

The Reflectance Prototype was a test jig to take basic measurements off a surface to determine requirements for a borehole configuration. These were used to determine the requirements for the reflectance channel design of the integrated prototype.

The purpose of this prototype was to test the three main components (detector, filter, and LED) in a reflectance geometry with materials previously tested (Chapter 2). The expected result was to demonstrate the capability to match the predicted reflectance using the methods developed

in Chapter 5 and to provide recommendations for the integrated instrument. This testing utilized the Dexter S25 detector, the matching Thorlabs LED and filter for the 1.5 μm channel (Table 3-7).

Three materials were measured. These were the Spectralon, Nextel target, and calcium carbonate (CaCO_3) sample. The CaCO_3 sample was selected as an example mineral found on Mars (Table 2-2) The Spectralon and Nextel target were selected to bound the upper and lower voltage readings to set the 100% and 0% reflectance values, respectively. Given these were correct, the calibrated CaCO_3 voltage readings should generate a reflectance value that would match the predicted value based on the methods from Chapter 5.

Reflectance Prototype Design

The reflectance jig design is shown in Figure 6-17. In this design, spacing of the detector and 1.5 μm LED were constrained by both their physical dimensions as well as the physical dimensions of the filter. These were set with matching 10° angles of incidence and reflectance (orthogonally to the material surface). For this set of experiments, an improved pre-amplifier was installed on the detector (see section 6.8 for details).

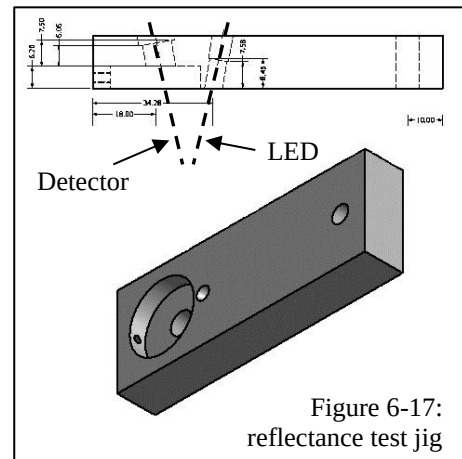


Figure 6-17:
reflectance test jig

Experiment

Methods

Configuration

The experiment was set up on the benchtop with no thermal control of the system beyond the room environmental control system and aluminium-mounting block.

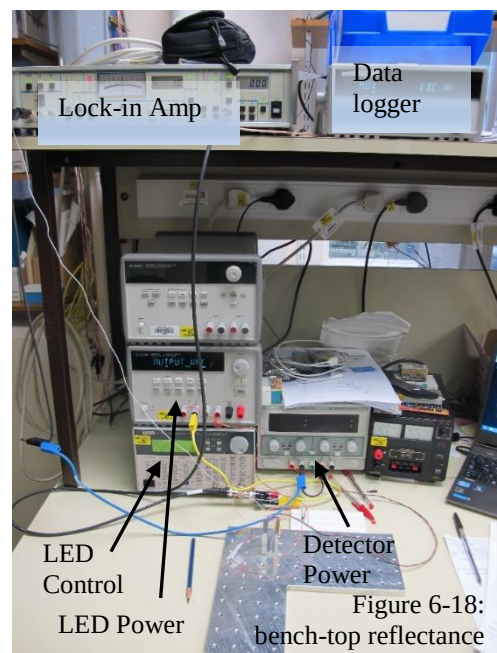
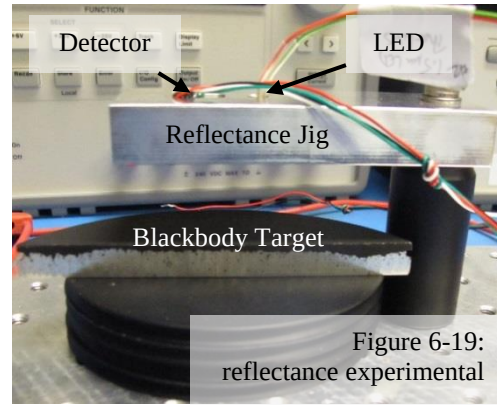


Figure 6-18:
bench-top reflectance

The bench-top experiment (Figure 6-18) included a number external support equipment. This equipment included: SR510 lock-in amplifier, Agilent data-logger, TTI function generator, and two power supplies (one to power the detector and one to power the LED).



Thermal background variations were eliminated with a chopped signal by electronically modulating the output from the LED with the TTI function generator. The SR510 lock-in was used to demodulate the chopped signal.

The experimental setup is shown in Figure 6-19. The top of the samples were set to a common height of 39.5 mm above the surface of the optics bench to ensure that they all had the same optical path from LED source to detector. The pre-amplifier from the Thermal Prototype II (Section 6.2) was used for this set of tests.

Table 6-6: Prototype II Support Equipment Settings

Protocol

The detailed protocol was 10 cycles of turning the LED on for 10 minutes and then off for 5 minutes. The settings for these experiments are provided in Table 6-6.

Equipment/Feature	Settings
Agilent (LED Power):	1.14 VDC
Tenma (Detector Power):	±15 VDC (dual power mode)
<u>TTI Function Generator</u>	
Frequency:	65 Hz
EMF:	+ 5 VPP
DC Offset:	+ 2.5 V
Symmetry:	50.0%
<u>SR510 Lock-in Amplifier</u>	
Signal Filters:	Bandpass-out, line-out, line-2X
Signal Inputs:	A, AC
Sensitivity:	2 x 10 mV
Dynamic Range:	Low
Display:	X
Expand:	X1
Time Constants:	100 ms
Post:	0.1s
Reference:	F; sine; Hz
HP data logger	1 s intervals, time, and date.

Calculations

The raw data were converted to individual cycle data by averaging the stabilized voltage readings. About 15 s of data were excluded at the start and end of each “LED On” cycle to avoid

the transition data. These were plotted against the average of all data points from all 10 cycles with a 1-sigma standard deviation.

These average values were converted to reflectance by a two-point calibration method normalizing measured voltages for samples to those generated for the Spectralon (98.7% reflectance) and the Nextel painted greybody target (11.8% reflectance). The method for the calculation of reflectance is provided in Equations 6-1 and 6-2.

$$\text{Reflectance} = \frac{\text{Voltage Sample} - \text{Voltage (greybody reflectance)}}{\text{Voltage Spectralon} - \text{Voltage (greybody reflectance)}} \quad \text{Equation 6-1}$$

Where the greybody reflectance is calculated from Equation 6-2 as follows:

$$\text{Voltage greybody Reflectance} = \frac{\text{Voltage greybody} - (\text{greybody Reflectance})(\text{Voltage Spectralon})}{1 - \text{greybody Reflectance}}$$

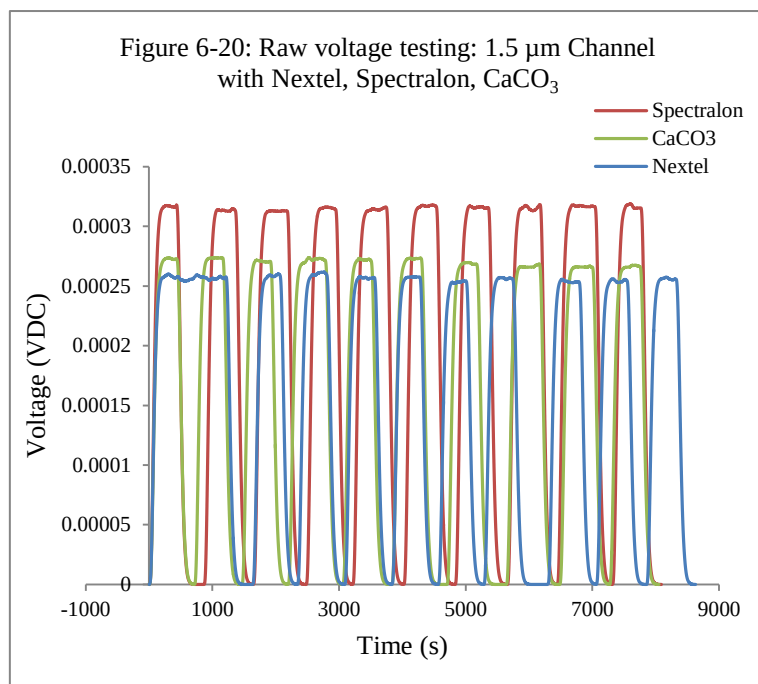
Results

Each of the three materials were measured independently. These are plotted in Figure 6-20. The individual cycle averaged data are plotted in Figure 6-21. The cycle averages are plotted by material type in Figure 6-22. The converted reflectance values are plotted in Figure 6-23.

Discussion

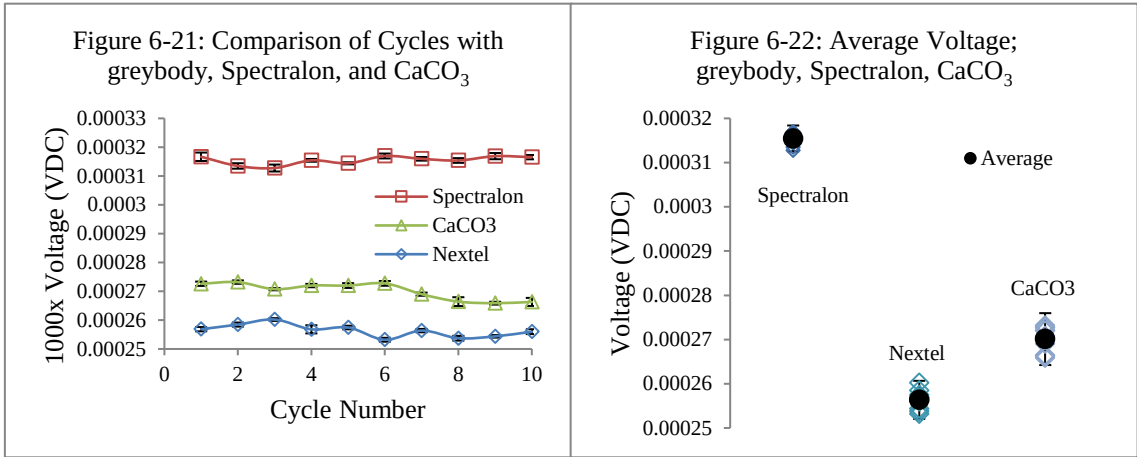
Results

In this test, three materials were measured with the 1.5 μm channel (Figure 6-20). The culmination of these tests demonstrated that the components as assembled could successfully measure the reflectance of a material and which matched the predicted results.



As was expected, Spectralon had the highest generated voltage, the greybody target had the lowest, and the CaCO_3 was in-between. Each sample showed good repeatability across the cycles with low variability within a cycle (0.6 to 1%).

Each individual cycle average is plotted in Figure 6-21. The 1-sigma standard deviation represents the electronic signal variability of all 10 cycles plotted in Figure 6-22.

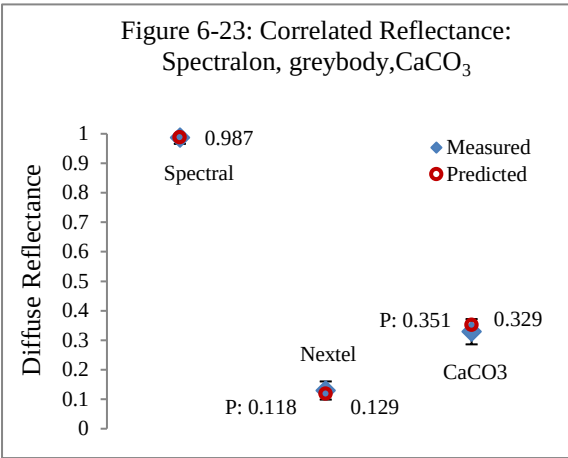


These values were converted into reflectance in Figure 6-23 using equations 6-1 and 6-2. Spectralon had the highest value, which was set to a reflectance of 0.987. The Nextel painted greybody was re-measured in the spectrometer and updated with a reflectance of 0.118 due to additional

degradation of the surface (dust, dirt, oil, etc.). The resulting measured value for CaCO_3 was 0.329, which is very close to the predicted value (denoted in Figure 6-23 with a “P”) of 0.351 and fell within 1-sigma standard deviation of the measured values.

Experimental limitations

This experiment was limited by the physical constraints of the filter. The optical path from the surface to the detector was about 20 mm, which was more than twice the specified distance for the integrated instrument of 8 mm. Because energy attenuates by the inverse square



of the distance, it is important to locate the detector as close to the surface as possible in order to maximize the flux reaching the detector.

The 25 mm diameter filter was the biggest limitation in this design. In order to reflect the LED IR radiation off the material surface, there needed to be enough separation between the detector and the LED to accommodate the filter. The best design would be to have matching angles of incident and reflectance with a filter orthogonal to the detector surface. The filter is a multilayer sandwich designed to allow the correct transmission characteristics and assumes that the light passes directly through the filter. Any angle would increase the transmission path through the layers and potentially change the transmission characteristics; therefore, it was important to keep the angle as close to orthogonal to the filter surface as possible. The 10° angle was a compromise to balance the need to have the filter and a reflectance angle.

Experimental assumptions

There were some key assumptions for this set of testing. First, it was assumed that the outer dimensions of the LED and detectors did not vary so that all LEDs and detectors would fit into the rig the same and allow the correct alignment. Variations in the alignment due to variations in the LED or detector outer dimensions would mean that less energy would be reaching the detector. The manufacturing tolerances were 0.1 mm for the LED hole. The distribution cone of the 1.5 μm was $\pm 5^\circ$ around the central axis. The 0.1 mm tolerance translates into an off-access angle error of 0.0025° or 0.05% error.

The second assumption was the inclusion of filters in the original concept in order to reduce the spectral confusion error (Section 1.6); however, including these significantly reduces the energy reaching the detector to about 1% compared to with no narrowband filter. This decreases the SNR while reducing the capability to discriminate the differences in percent concentrations due to a smaller dynamic range. The two ways to improve this are to eliminate the filter and/or to increase power to the LEDs. Eliminating the filter would significantly increase the energy reaching the detector by as much as 2 orders of magnitudes, but would increase the spectral confusion because of the wider range of frequencies associated with the spectral characteristics of the LEDs without the filter.

The other option is to increase the power to the LEDs. This would increase the forward optical power and increase the energy reaching the detector. The LEDs typically have a 100% duty cycle limit of about 150-200 mA in order to prevent over-heating. Pulsing the LEDs allows it to cool and the power can be increased significantly. This is an advantage because the lock-in amplifiers require a pulsed signal; however, these have a minimum duty cycle that can be detected.

The specifications for the Deep Red Technologies LEDs (1.95 and 2.05 μm , Figures 3-21 and 3-22 and Table 3-5) call for a pulsed duty cycle of no more than 1%, but allows the power to be increased to 1 amp. This increases the forward optical power from 1 mW to 25 mW (25x increase). The other LEDs are similar in performance.

The minimum duty cycle for the SR510 and SR830 as tested were 20% and 3%, respectively. Any increase in the duty cycle will require a reduction in the supply power to the LED. The reflectance calculations in Section 5.4 assumed the maximum forward optical power allowed under a 1% duty cycle. The reflected energy from the ISBG 1.93 and 2.05 μm LEDs are already at the detector threshold with the assumed 1% duty cycle power value, so this reduction in the assumed forward optical power could have a significant impact on the instrument performance. This is tested and discussion in Section 6.9.

Experimental errors

The one minor source of error in this experimental design was due to the electronics. For this set of experiments, an improved pre-amplifier was installed on the detector (see section 6.5 for details). Results were stable as indicated in figure 6-20. This noise shows up as the small-scale variability across each set-point, or the standard deviation. The scale of this variability was the same with or without the filter, confirming this was noise in the electronics. This was less than 1% without a filter, but accounted for ~5% error with a filter.

Conclusions and recommendations for an integrated prototype

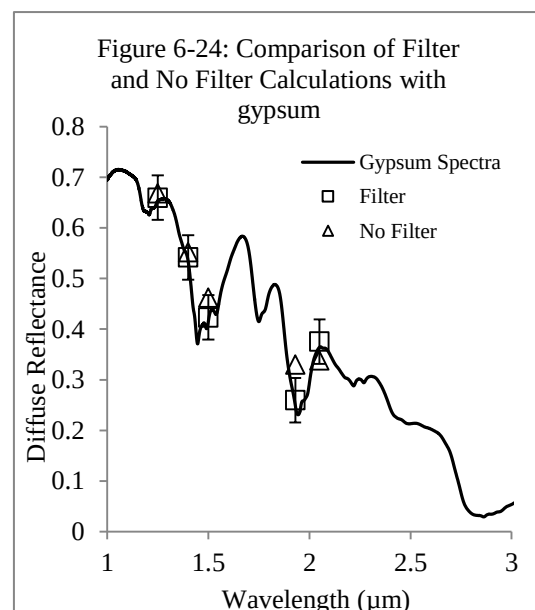
The measured reflectance was demonstrated to match the predicted result for a pure sample of CaCO_3 in the 1.5 μm channel. This was accomplished with completely commercial off the shelf components and benchtop electronics. The final step in this project is to build an integrated instrument in a full borehole geometry with both the thermal and reflectance channels. A number of recommendations are made for the integrated design from the results of the reflectance testing. This is in addition to recommendations made at the end of Section 6.4

- Use a single detector for thermal and reflectance channels
- Determine if the filters can be eliminated and if not, if they can be placed in front of the LED to accommodate a single detector design
- Boost the power to the LEDs
- Reduce the signal noise by co-location of the pre-amplifier and lock-in amplifier as close to the detector as possible
- Utilize a geometry with the detector surrounded by the five LEDs

6.6 Filter Analysis

Elimination of the filters would be highly desired as this would simplify the design and because custom filters are costly. This had to be balanced against the science requirements. Three different design solutions (1-3) of filters and LEDs were considered with 3 different configurations (A-C). The pros and cons of each of these were determined. The summary of this analysis is provided in Table 6-7.

Design solution 3, no filters and a single detector, has the key advantage of significantly higher levels of reflected energy reaching the detector (e.g., increased SNR). The key



disadvantage is that there will be increased spectral confusion because of the wider spectral characteristics of the LED as the radiation source. This will lead to a higher error for the detection and discrimination of percentages of mixed minerals.

Table 6-7: Filter/LED Design Solution Analysis

Filter/LED Design Solution	Pros	Cons	Allowable Design Configurations
1 - Filter for each band - LED - No temp control - Temp measurement of lamp	- Filter tuned to specific required absorption band - No need to control temp of LED - Could replace detector window (KRS-5) with filter in 1 det/filter design - Increased transmission - Increased SNR	- Need to have well characterized temp dependent spectral characteristics of LED - IR reflected energy not maximized - Decreased SNR - Additional filters reduce transmission to detector in 'B' configuration - Decreased SNR - Increased complexity of system - May require 1 detector for each filter ('A' Configuration).	A 1 detector for each filter/LED - Multiple units along length of probe string B 1 detector with KRS-5 window - Multiple LED - Filter feeder in probe string
2 - Filter for each band - LED - Temp control - Temp measurement of lamp	- Filter tuned to specific required absorption band - Less reliant on temp dependent spectral characteristics of LED - IR reflectance energy maximized - Increased SNR	- Increased complexity of additional thermal control for each LED - May not be possible to have multiple LED config 'B' - Additional filters reduce transmission to detector in 'B' configuration - Decreased SNR	A 1 detector for each filter/LED - Multiple units along length of probe string B 1 detector with KRS-5 window - Multiple LEDs - Filter feeder in probe string
3 - No filter for reflectance bands - LED - Temp control - Temp measurement of lamp	- IR reflectance energy maximized - Increased SNR - Less complex design because fewer filters - Increased transmission - Increased SNR	- Completely reliant on LED temp dependent spectral characteristics - Must control LED temp - Increased complexity of additional thermal control for each LED - May not be possible to have multiple LED config 'B' - Not using tuned filter to cut tails from LED spectral curve - If 1 LED/det config required, then better to go to config '2.A'	C 1 detector with KRS-5 window - Multiple LED <u>NO</u> reflectance band filters on feeder

This is demonstrated in the example of pure gypsum in Figure 6-24. In this figure, the integrated reflectance for the Filter and No Filter configurations were calculated for each channel, with the Filter configuration representing the original assumption that a filter would be necessary.

As was previously shown in Figures 5-12 and Figures Appendix A-1 to A-4, the integrated values are dependent upon the slope of the material spectral characteristics within the bandpass (this was previously demonstrated in Figure 5-14 with filters). If there is a large slope, the integrated value may not align with the desired peak reflectance feature. The rates of error will vary by channel, so it may be that some channels will have sufficient accuracy without the filters while others may need a filter. This is clearly demonstrated in Figure 6-24. The 1.93 μm band where the No Filter configuration has an integrated reflectance well outside of the error of the Filter calculation; the 1.5 and 2.05 μm channels just fall within the error bars; and the 1.25 and 1.4 μm channels are well aligned with each other. This example provides a worst-case example of all of the minerals examined, though each mineral will have different rates of error across the bands.

The percent difference between the expected Narrowband calculation as the baseline and the Wideband calculation is provided in Table 6-8 for each of the pure minerals previously considered. The minimum and maximum difference

Table 6-8: Percent difference Filter to No Filter

Sample	Channel Percent Difference: (Narrow – Wide)/Narrow				
	1.25	1.4	1.5	1.93	2.05
CaCO ₃	0.61%	1.22%	1.20%	2.66%	1.65%
Basalt	0.71%	0.71%	0.70%	3.01%	0.71%
CaCO ₃ w/Fe	3.91%	0.52%	0.00%	1.04%	0.76%
Limestone	0.30%	0.78%	0.80%	6.18%	1.60%
Gypsum	1.36%	1.85%	9.22%	26.92%	9.87%
SiO ₂ – Fisher	1.52%	0.45%	0.15%	1.07%	0.75%
SiO ₂ – Acros	1.82%	2.44%	0.00%	1.03%	0.57%
Jarosite – RT	1.36%	3.91%	0.58%	3.86%	1.22%
Jarosite – Ca	1.21%	7.07%	3.43%	0.98%	1.04%
Halite	1.98%	0.27%	0.81%	1.31%	1.02%
Montmorill.	1.07%	4.26%	0.35%	1.23%	1.36%
Min	0.30%	0.27%	0.00%	0.98%	0.57%
Max	3.91%	7.07%	9.22%	26.92%	9.87%
Average	1.44%	2.13%	1.57%	4.48%	1.87%
Stdev	0.96%	2.14%	2.71%	7.62%	2.68%

in each channel is noted as well as the average channel difference with the standard deviation.

As noted in the Figure 6-24, gypsum was the example with the largest differences, especially in the 1.93 μm channel that resulted in almost 27%, but also nearly 10% difference in the 1.5 and 2.05 μm channels. The channel averages, not counting the 1.93 μm channel, are less than $2.15 \pm 2.68\%$, with the 1.93 μm resulting in $4.5 \pm 7.6\%$. Removing gypsum drops the 1.93 μm to $2.2 \pm 1.7\%$ average max error.

From the analysis of the data in Table 6-8, it is confirmed that the elimination of the 1.25, 1.4, 1.5, and 2.05 μm filters will add an estimated 2% error. Given the trade-off between cost and performance, this seems an acceptable trade. The 1.93 μm channel results indicate that a filter is necessary. This presents a difficult problem in terms of channel performance vs. the cost and added complexity for adding a custom filter. As was noted in Appendix Tables B-3 and B-4, the 1.93 μm LED has the lowest forward optical power, resulting in the lowest performance. These tables calculate the channel performance with a filter, but the results show that the performance is on the low side. Eliminating the filter would significantly increase the forward optical power reaching the detector and the SNR, but at the cost of a significant increase in the error.

For this integrated design, it was recommended to not include filters in any of the channels, but to prepare the 1.93 μm channel with the spacing to accommodate a custom filter placed in front of the LED in the future if funds became available.

6.7 Integrated prototype development

The purpose of the integrated prototype was to design and test a technology demonstration of what an integrated Mars instrument might look like. There were a number of recommendations made in both the thermal (Section 6.4) and reflectance (Section 6.5) prototypes as well as some additional limitations identified during the design of this instrument. The original concept was presented in Figure 1-7. This concept had a detector, LED IR sources, filters, and the electronics in a borehole configuration looking out to the side. Multiple channels were expected to be accommodated by individual detectors mounted along the length of the device, or by a multi-element single detector with filters over the different elements for the channels. A summary of the key recommendations affecting the physical design of the instrument is as follows:

- Have a single element detector with the 5 LEDs surrounding it
- Provide active and passive thermal control for the detector and LEDs
- Keep thermal control of the detector to within ± 100 mK of specified set-point

- Co-locate the pre-amplifier and lock-in amplifier as close to the detector as possible
- Determine if the filters can be eliminated in the design

In addition to these recommendations, there were a number of outstanding issues that needed to be resolved during the final design development. These included the following:

- Determination of location of the power supply: co-located in the bore-hole device or external at the surface
- The micro-controller selection was previously identified as an Arduino micro, but this needed to be re-assessed during the design of the electronics boards
- Selection of an external support computer and development of a basic User Interface
- Eliminate all filters, scar for 1.93 μm future filter

A physical design was then made and then the integrated electronics were developed to provide the four key PCB boards. This is detailed in the following sections.

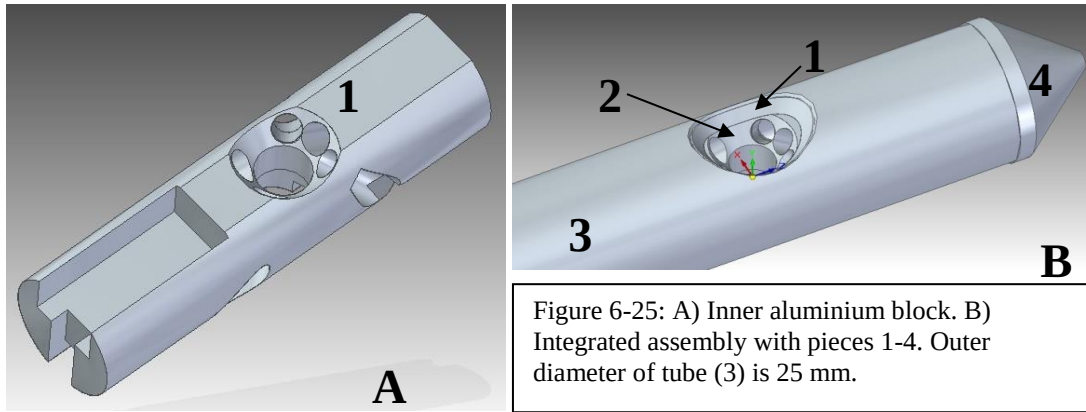
6.8 Instrument Detailed Design

The block diagram (Figure 6-1) shows a number of major subsystems in the integrated design. The key design features have a centrally located detector surrounded by the five LEDs. These were embedded in a thermal block with active heating and passive cooling. Two additional layers provided both isolation and insulation. The various subsystems are described in the following sections.

Mechanical

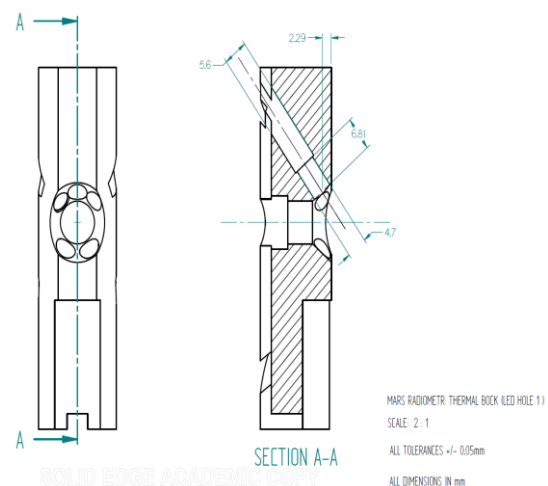
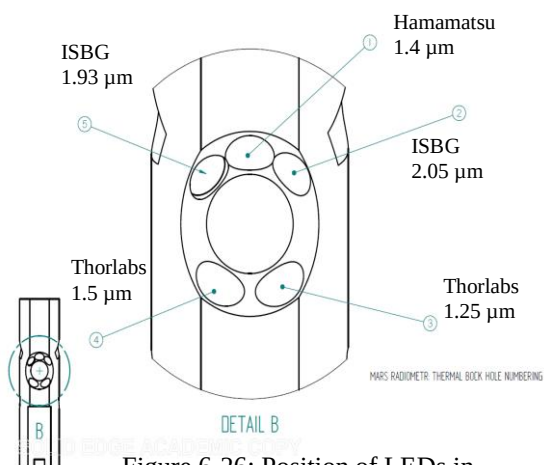
The mechanical block followed the same multi-layer design concept as the Thermal Prototype (Figure 6-6) and has 4 primary sub-components (Figure 6-25 A and B):

- 1) Inner thermal control block. This is aluminium 7075 that holds the detector and all the LEDs. It was sand blasted and hard-coat anodized black. The temperature of this block is actively maintained with a thermocouple and a ceramic heater. The detector and LEDs were mounted to this block.



- 2) Thermal Insulation Layer: This is made of PTFE plastic that serves as a thermal break between the outside environment and the thermal control block.
- 3) Outer layer: This is a stainless steel tube that contains the assembled system including the thermal control block with detector and LEDs, thermal insulation layer, and control electronics with the Arduino Micro.
- 4) An end cone that prevents dirt or other items from entering into the tube (aluminium 7075).

Internal details of the Aluminium block are provided in Figures 6-26 and 6-27. The five LEDs are mounted along the centreline of the length. The two largest diameter LEDs (Thorlabs 1.25 μm and 1.5 μm) are mounted on one end while the TO-5 can style LEDs (Hamamatsu 1.4 μm and ISBG 1.93 μm and 2.05 μm) are mounted on the other side. The dimensions of the internal layout are shown in the cut-away view in Figure 6-27. This shows how the detector is recessed from the surface. A 30 degree off-set angle positions all the LEDs at the same angle in relation to the centreline of the detector. They are offset to the edge of the detector such that the detector



cannot see any of the LEDs directly. This design allows the light from the LEDs to be reflected off the material surface into the detector even if the integrated instrument is completely up against the surface. One limitation in this design approach is that in order to accommodate 5 LEDs, the angle of incidence (30° orthogonally to the surface) is not the same as the angle of reflectance; however, this will be accounted for by calibration with the Spectralon calibration target. A counter-sink was placed in front of the $1.93\ \mu\text{m}$ LED to accommodate a filter if/when possible. The fully assembled integrated instrument as built is shown in Figure 6-28.

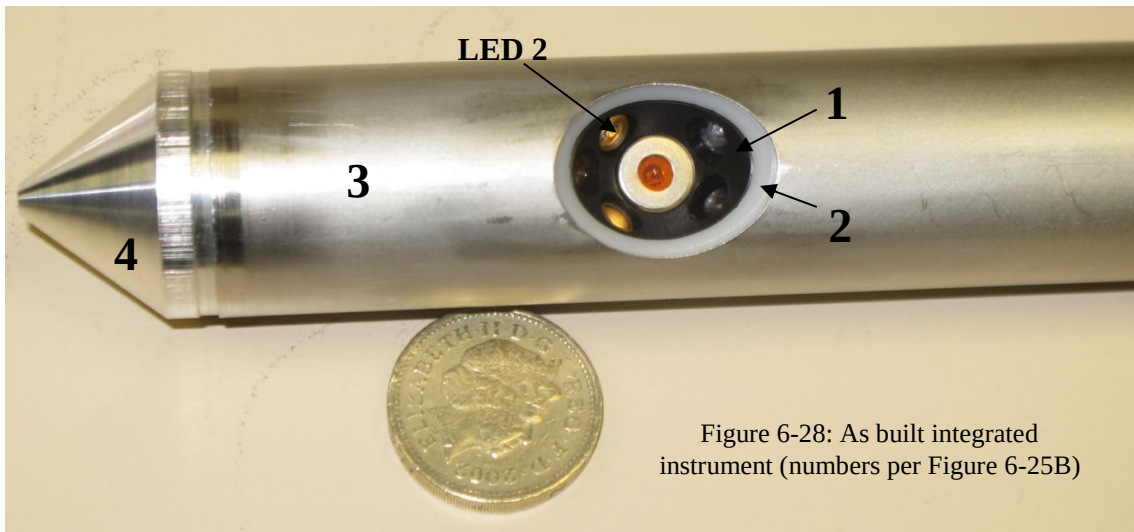


Figure 6-28: As built integrated instrument (numbers per Figure 6-25B)

Electronics boards

There were 4 main electrical boards that were developed in support of the field instrument. These were: 1) Pre-amplifier, 2) Bore-hole PCB with lock-in amplifier, 3) Arduino micro-controller with shield, and 4) LED control and power distribution board. The pre-amp and lock-in amp were located in the borehole, while the other two were located externally.

Pre-amplifier

A new design was required for the integrated instrument because of size limitations. The previous quad op-amp (AD470) was too big to fit behind the detector, so an AD8599 was selected as the replacement. This is an ultra-low noise ($1.1\ \text{nV}/\sqrt{\text{Hz}}$), dual op-amp (manufacturers' datasheet). The circuit is similar to the previous configuration (Figure 6-

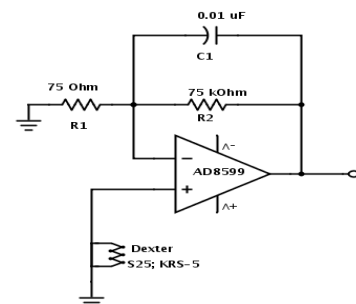


Figure 6-29: Pre-amplification Circuit

2) with the updated circuit provided in Figure 6-29. The integrated detector and pre-amp are shown in Figure 6-30. Testing of the device demonstrated a linear response with an amplification of 1000x.

Borehole PCB

The out-put signal from the detector pre-amplifier was sent to the Borehole PCB which included the lock-in amplifier circuit and additional circuitry necessary for the control of the bore-hole system including the thermocouple temperature sensor, a four-channel analogue to digital (ADC), and a digital to analogue converter (DAC). The as-built configuration is shown in Figure 6-31 with the full circuit provided in Figure 6-32. The signal from the detector is passed through the lock-in amplifier, when used in the reflectometer mode, to the ADC.

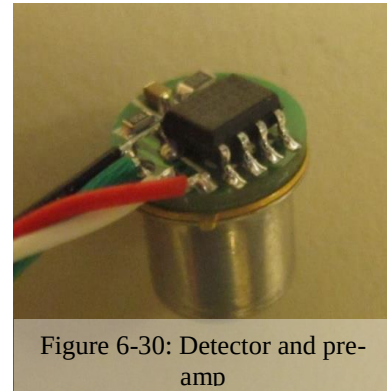


Figure 6-30: Detector and pre-amp

Figure 6-31: Borehole PCB

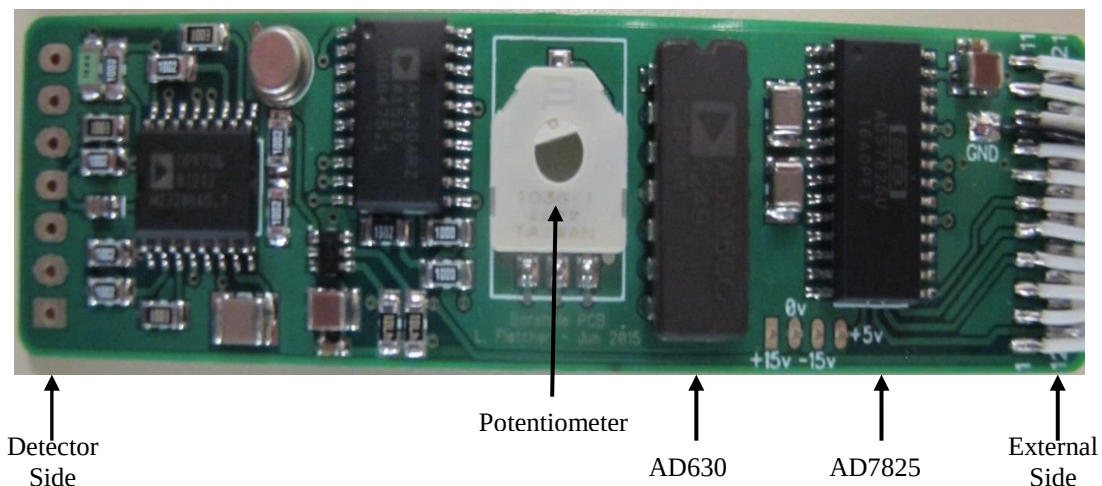
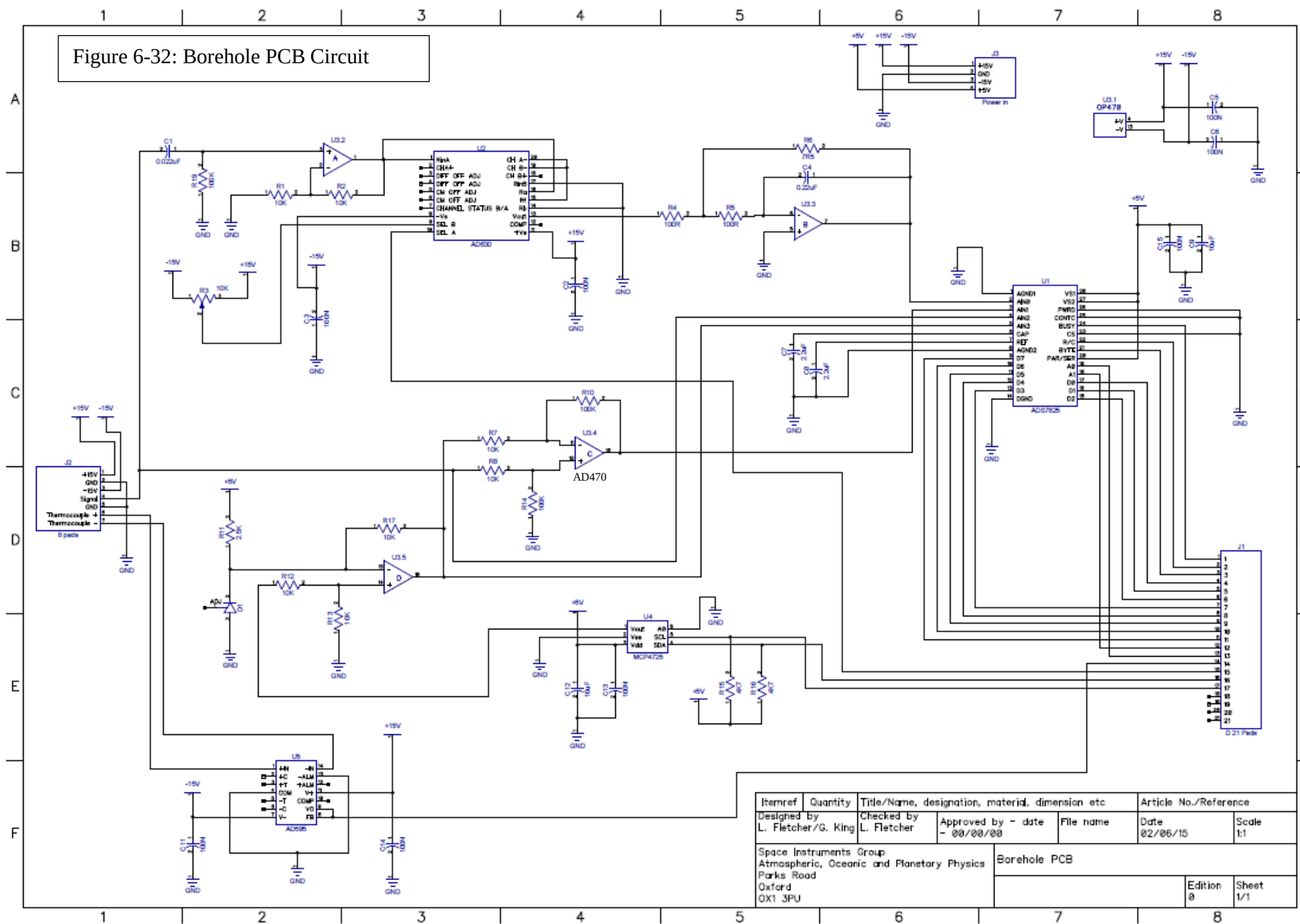


Figure 6-32: Borehole PCB Circuit



Itemref	Quantity	Title/Name, designation, material, dimension etc		Article No./Reference	
Designed by L. Fletcher/G. King	Checked by L. Fletcher	Approved by - date - 00/00/00	File name	Date 02/06/15	Scale 1:1
Space Instruments Group Atmospheric, Oceanic and Planetary Physics Parks Road Oxford OX1 3PU			Borehole PCB		
				Edition 0	Sheet 1/1

In the case of the thermal IR mode, the detector has a natural off-set voltage that varies with detector temperature. This is determined with calibration, but this off-set can significantly reduce the dynamic range of the amplified values if it is too large. To adjust this to a zero starting value at calibration, a digitally controlled, variable voltage adjustment circuit was included. The detector signal output from the pre-amplifier is measured directly to determine the offset voltage. This voltage value is then generated by an MCP4725 digital to analogue converter and subtracted from the pre-amplified output from the detector. This sets the calibration value with the blackbody target as close to zero as possible. This allows measurements to be amplified an additional 10x before being passed into the ADC. This increase in the dynamic range allows a more accurate scene temperature measurement. The other three channels of the ADC are used for the thermal IR mode to record the output signal directly from the pre-amplifier, the adjustment for the off-set voltage, and the off-set voltage adjusted and amplified signal.

Lock-in Amplifier

A principal feature to the performance of the reflectance channels is to be able to filter out a signal from the thermal background noise of the scene noise. A primary way to do this is to chop the signal at a specified frequency. The data will be collected only when the signal is high in phase. There are two ways to chop the signal in these applications: 1) physical chopping, and 2) electronic chopping. Physical chopping requires a mechanical means of interrupting the detectors view of the scene. This would require large moving or (ideally) rotating blades. The other choice is electronic chopping in which the signal is interrupted by turning the power to the LED on and off. In the borehole device, space is much too limited to accommodate physical chopping, so electronic chopping was selected as the choice to interrupt power to the LED. Data are collected while the LED is lit and ignored when it is off (for the reflectance channels).

A lock-in amplification circuit (Figure 6-33) was based off previous work (Garcia, 1988) using an Analog Devices AD630 as the central component. This is a phase sensitive, balanced modulator/demodulator that can be used to lock-on to a signal using an external reference. The first stage is an amplification stage that feeds into the AD630 (stage 2). An external controller

(the micro-Arduino in this case) provides the PWM on/off control of the LED as well as the reference in the second stage. The

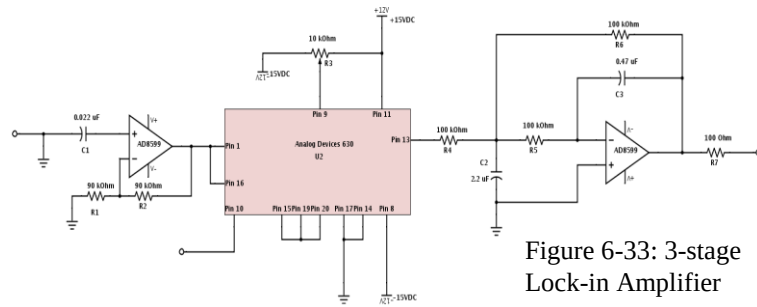


Figure 6-33: 3-stage Lock-in Amplifier

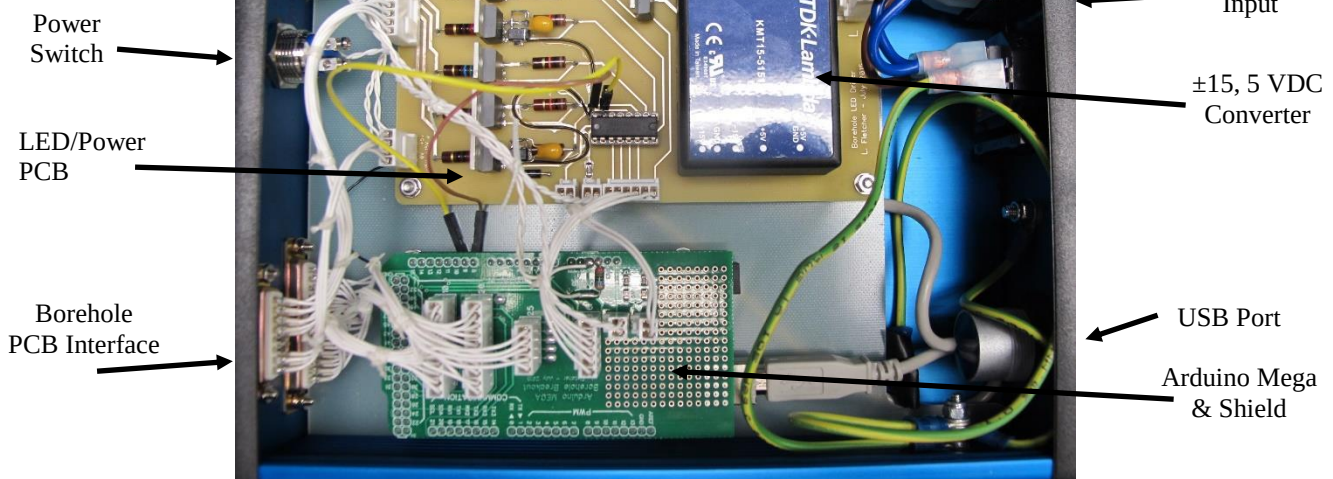
demodulated signal is then fed into the third stage, which is a low-pass buffer/amplifier. In the case of this design, the first stage is a 1x amplifier while the third stage provides a modest 15x amplification.

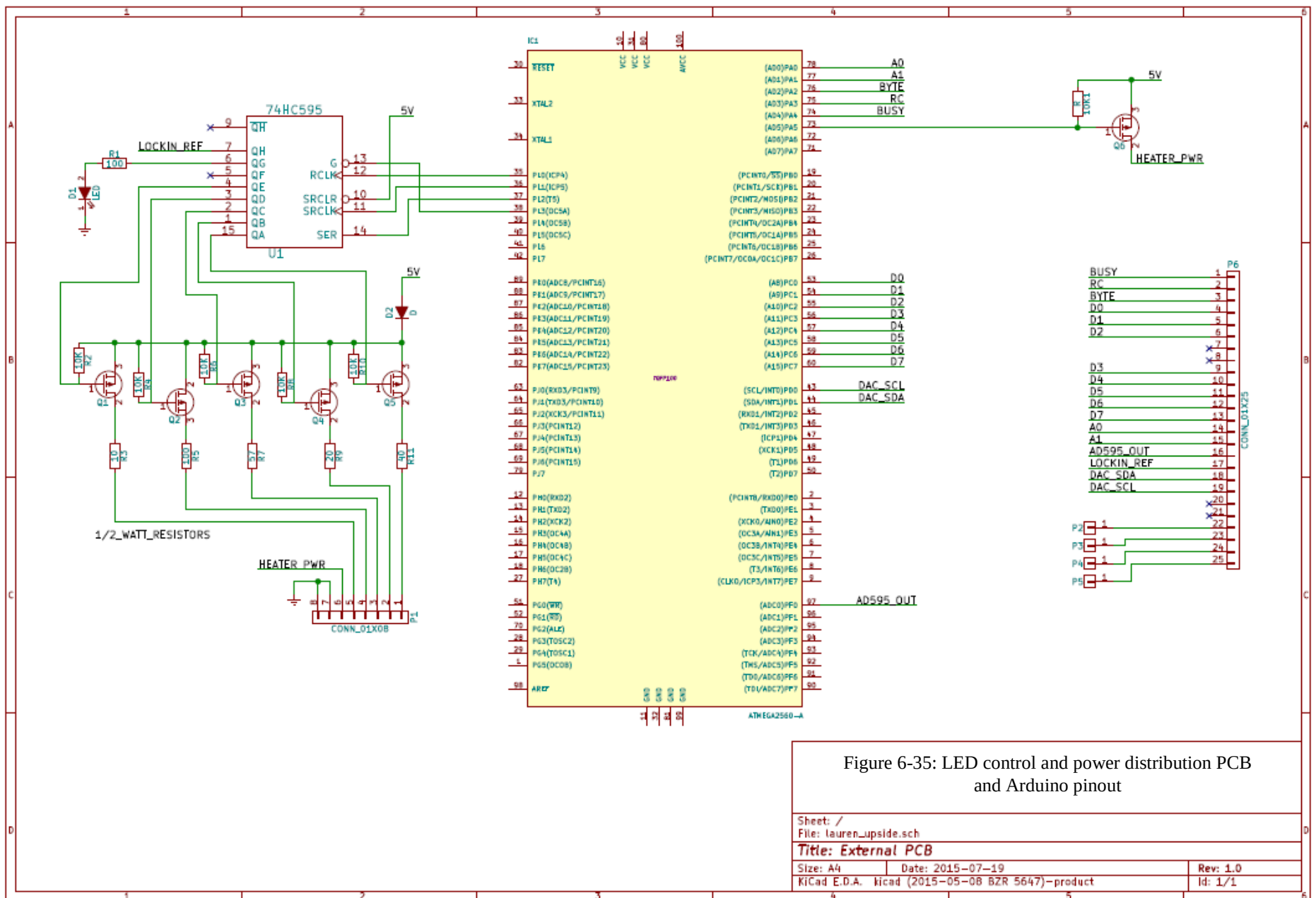
External Electronics

Two external boards were designed. The first was a shield for the Arduino Mega in order to provide the interface connectors to the other three boards (diagram not provided). The second was for the LED control and power conversion and distribution (Figure 6-35). The Arduino Mega and the two external boards were built into an aluminium box with an AC power input and a USB port (Figure 6-34).

The original intent was to have an Arduino micro (Figure 6-6) as the central micro-controller located in the borehole electronics. This was dependent upon the number of analogue and digital In-put/out-put channels that were required for all of the difference components. During the development of the borehole PCB, the total number of I/O channels required exceeded those

Figure 6-34:
external
electronics box





available on the Arduino micro, so a decision was made to switch to an Arduino Mega. Since the Arduino Mega is much larger than the borehole diameter, it was necessary to move this system to outside of the borehole. The LED control and power distribution components were also moved to outside the integrated instrument. These changes were necessary due to space limitations, but also had the advantage of moving significant heat sources away from the detector to allow better thermal control. A shield was designed to allow easy assembly and change of the mega in the case of a failure. The USB port was connected to the Arduino Mega to allow control and data collection from an external computer.

Arduino Mega and Control Code

The Arduino Mega served as the central microprocessor of the integrated system. This interfaced with and controlled the LEDs, data signals, thermal control system, and to the external support computer. The Arduino Mega pinout is provided in Figure 6-35.

The reflectance and thermal signals from the detector are converted by the ADC (AD7825) and then are passed to the Arduino Mega, which writes the data to a file on an external support computer including the time-stamp and other data as required. The Arduino Mega controls the LED pulsed signal through an 8-bit shift register (Texas Instruments 74HC595). This allows each of the LEDs to be controlled individually. A thermocouple amplifier with cold junction (AD595) serves as the interface to the K-type thermocouple mounted in the aluminium block. The Arduino Mega uses PID control with that signal to control the temperature of the block according to the requirements of the target environment.

The integrated system code was written in C and designed for the ATMEGA 328P to provide basic hardware control and interface to the borehole instrument. User control was via a python script run through a python prompt window on the external PC. This allowed the user to turn on and off individual LEDs, and collect and record data. All four channels coming from the ADC were recorded, so thermal IR and IR reflectance data could be collected simultaneously. Data were output to a user named comma-separated-value (.csv) file. This was connected to an external PC.

6.9 Integrated prototype benchtop testing

The purpose of this testing was to demonstrate the capability of the integrated prototype (Figure 6-28) to measure the reflectance off of a material surface and to compare the measured results to the predicted values. Testing was in two steps. The first was to test the integrated instrument with the benchtop electronics. The use of the benchtop electronics in this step was to eliminate error associated with the custom electronics. The second step was to repeat step one tests with the custom electronics.

Testing with benchtop electronics

Method

This testing followed the methods used in Section 6.5. The instrument probe was placed directly on the material surface with the detector as close to orthogonal as possible. Data were collected for all five channels before changing material.

The benchtop electronics setup was similar to the previous testing with the exception of changing the SR510 for an SR830 digital lock-in amplifier. The settings for these were determined from the Spectralon measurement and were specific to each LED/Channel. The sensitivity settings on the SR830 and duty cycle and pulse frequency on the TTI function generator were balanced with the objective to optimize the amplification range of the lock-in. The specific settings for the LED/Channel were used for all subsequent measurements in that channel.

The experiment protocol ran three tests for each material. Each test had three on/off cycles of the LED. Each cycle duration depended on the time constant setting on the lock-in amplifier. With a 1 second time constant, cycle times were 1 minute on and 1 minute off. With a time constant of 1 minute, cycle times were 5 minutes on and 5 minutes off. A two-point calibration was first run with the Spectralon and Nextel targets, and then the samples were run.

All data points from the 9 replicates were included in the average and standard deviation. Data beyond 2 sigma from the original set were excluded. These data were used with Equations 6-1 and 6-2 to determine the reflectance values. These were plotted in relation to a linear fit of the two-point calibration between Spectralon and Nextel and included the predicted values from

Chapter 5. The measured and predicted values for the samples were then plotted against the spectra.

Results

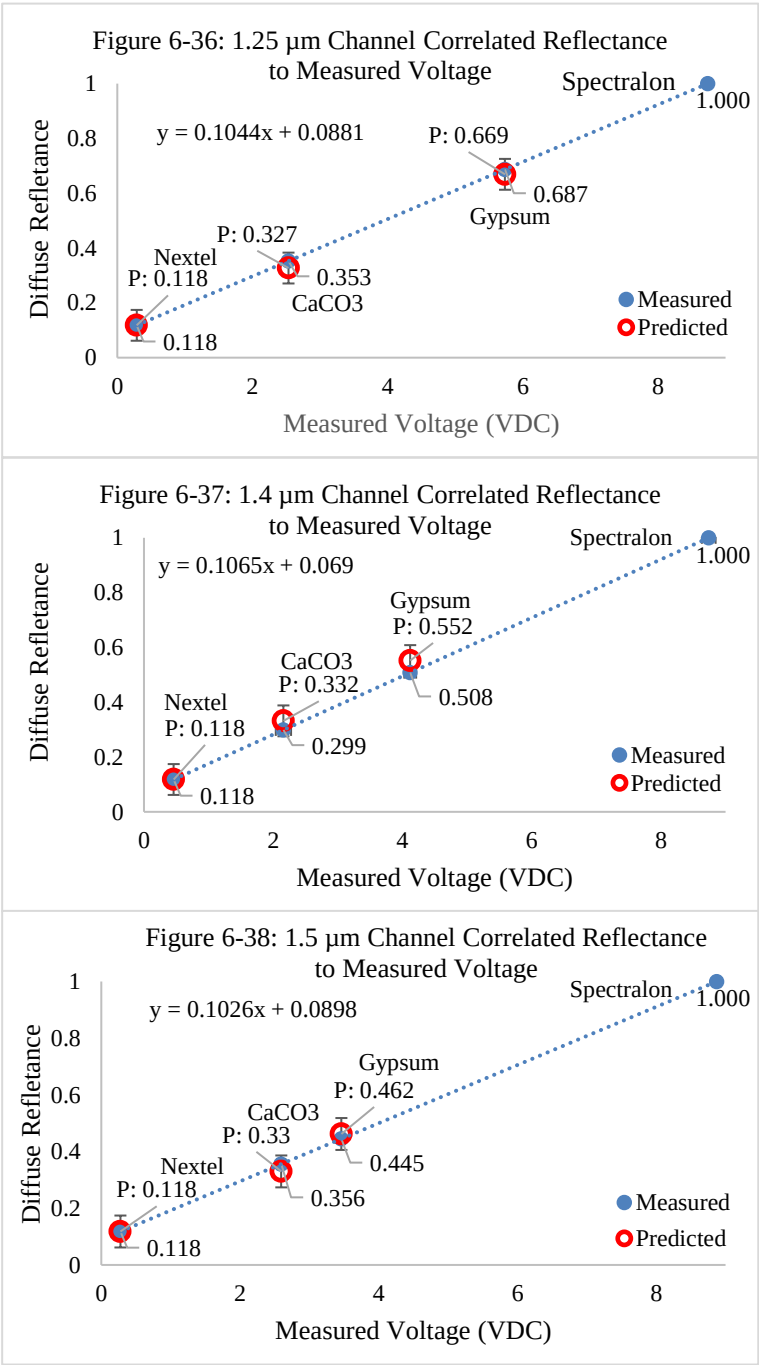
The results for each channel are provided in Figures 6-36 to 6-40. Figures 6-41 and 6-42 plot the results against CaCO_3 and gypsum spectra, respectively.

Discussion

The central result to these tests are that the measured results fell within the 1-sigma bounds of the predicted value in all channels for both minerals, when normalized to Spectralon and the Nextel painted target. The allowable error for the predicted value was $\pm 6.1\%$ (root-mean-square of sources of error). The error for the actual measured results was

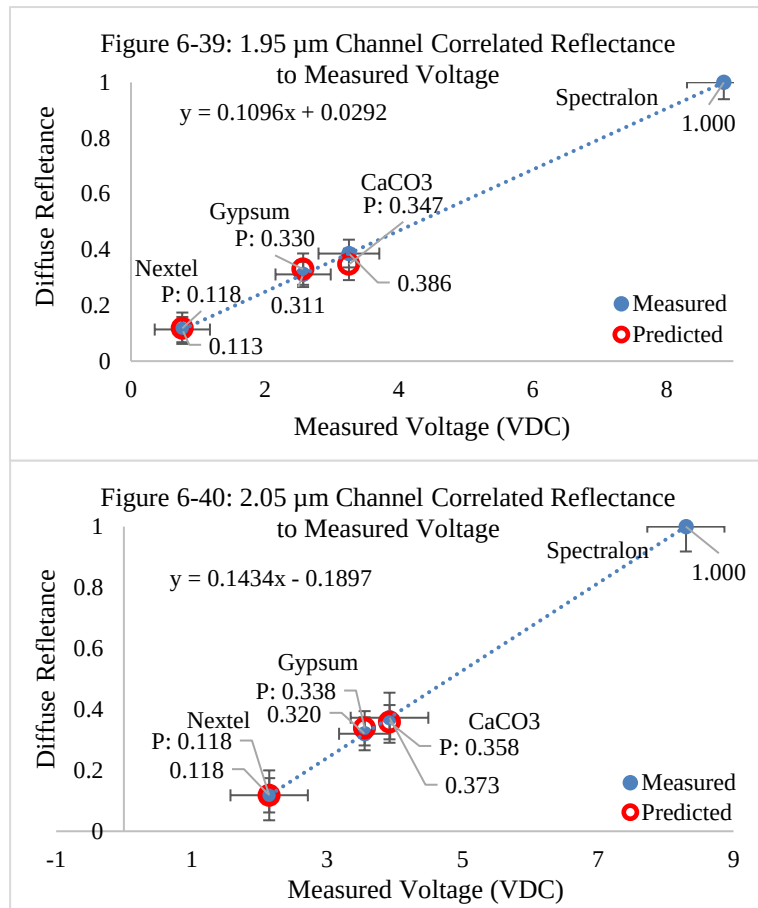
typically about $\pm 2.5\%$, based on voltage variation.

There are a number of errors that will have impacted the measured values. These were previously described in Chapter 5 for the predicted error analysis and are summarized in Table 6-9. The error bars for the predicted values include these sources of error.



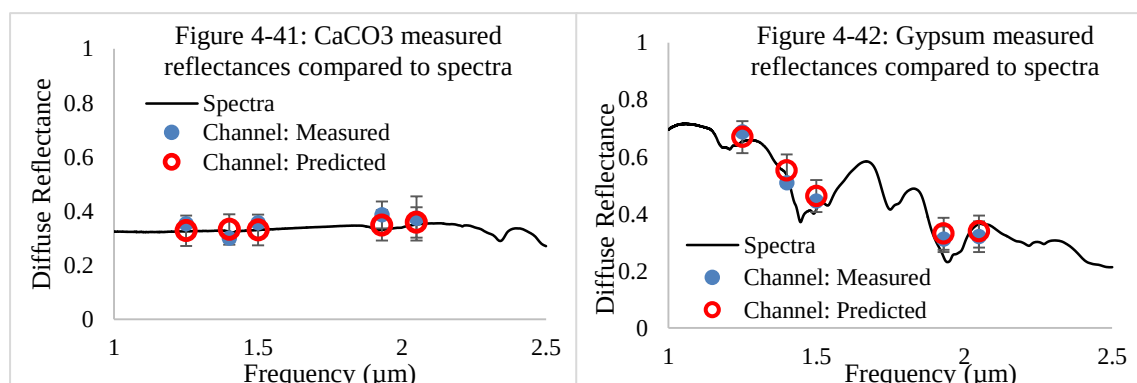
One additional form of error that was specific to this set of testing was related to the geometry of the experiment.

The position of the detector must be orthogonal to the surface in order to optimize the LED energy reflected towards the detector. In this set of experiments, the instrument was placed on top of a flat surface of a sample, but there was some variation



in the position during the change of samples. This could have amounted to an error of a couple of percent relative reflectance, accounting for nearly the entire difference from the measured to the predicted values. In a borehole, the probe will be extended down the length and will always keep the detector orthogonal to the measured surface, so this form of error is expected to be eliminated.

The 1.4 μm channel measured values were lower than the predicted for both samples. This is attributed to the original predicted calculations, which assumed a power distribution by the spectral distribution of the LED. Previously it was noted that manufacturers' data could have deviation from the as-built hardware. This is the likely cause, accounting for an additional



measured error of a couple of percent relative reflectance. Having a better measurement of the forward optical power of the as-built component would help improve the model calculations.

This test successfully demonstrated that the measured results could match the predicted results for two samples in five channels with an error of about $\pm 2.5\%$. The final test will repeat this with custom electronics.

Testing with custom electronics

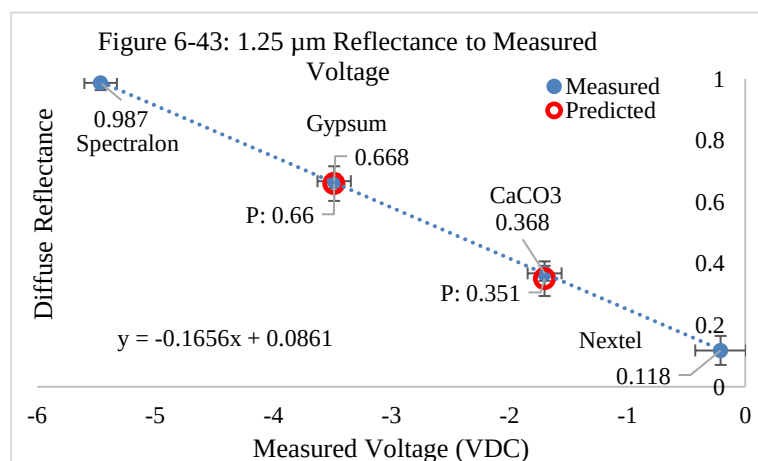
The previous test with the benchtop electronics was repeated with the custom electronics. The expected result was to demonstrate the capability to match the predicted reflectance using the methods developed in Chapter 5.

Method

This testing followed the methods used in in the previous section excluding the benchtop electronics. The geometry and protocol was repeated in this testing. One minute of data were collected in each On/Off cycle. As previous, the 9 replicates of data were used to calculate the average and standard deviation. Data more than 2 sigma from the original average were excluded.

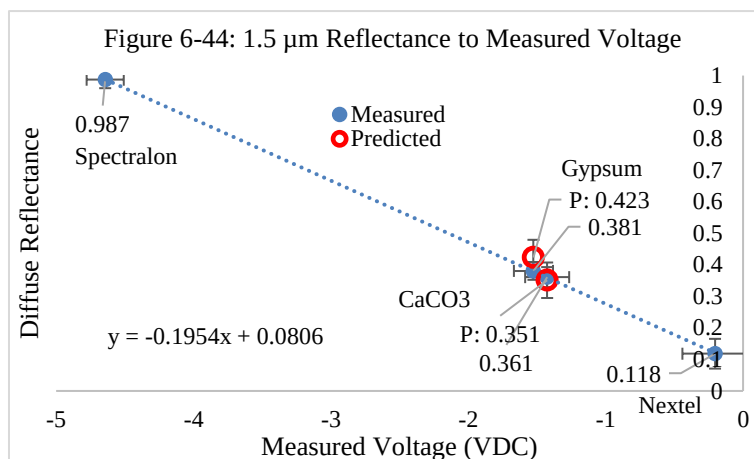
Results

The results of testing in this experiment are provided in Figures 4-43 and 4-44 for the 1.25 and 1.5 μm channels, respectively. There were not sufficient results to produce figures for the 1.4, 1.95, and 2.05 μm channels.



Discussion

The central result to these tests are that the measured results fell within the 1-sigma bounds of the predicted value for the 1.25 and 1.5 μm channels for both



minerals, when normalized to Spectralon and the Nextel painted target. The allowable error for the predicted value was $\pm 6.1\%$ (based on RMS error analysis of the various sources identified in Section 6.10). The error for the actual measured results was typically about $\pm 3\%$, based on voltage variation.

However, the results of this testing were incomplete with no results produced for the 1.4, 1.95, and 2.05 μm channels. In these channels, the data were effectively noise for all of the samples. There was not enough reflected energy for demodulation when compared to the background noise. The reflected energy is dependent upon the forward optical power. In the design of the custom electronics, the minimum duty cycle that was registered by the lock-in circuit was 33%. The allowable duty cycle for the maximum applied current to the IBSG LEDs (1.95 and 2.05 μm), was 1%. By going from 1% to 33% duty cycle, the power supplied to the LEDs had to be significantly reduced. This directly reduced the forward optical power. The resulting reflected energy was not sufficient to be discriminated in the signal noise with the custom electronics. This was the same result for the 1.4 μm LED.

One of the design flaws in the electronics is the static amplification. In the original calculations, a minimum amplification range was determined that would allow the discrimination of the signal in the lower power LEDs (1.4, 1.95, and 2.05 μm), but assumed a 1% duty cycle. This was fixed as a static value in order to simplify the electronics design. This was an error as subsequent testing required a reduction in the current supplied to these LEDs and the assumed amplification was rendered insufficient. It is possible that a dynamic gain circuit would solve this problem in future designs.

6.10 Systematic Error Analysis

A number of sources of error have been discussed and presented throughout the thesis, in particular, Section 5.7. Testing in this chapter provided the final measured system error in the thermal channel B (Table 6-4) and the reflectance channels (Section 6.9). The systematic error was calculated as the root-mean-square (RMS) of all of these identified errors. These are summarized in Table 6-9. The details are provided in Appendix E.

Table 6-9: System RMS Error by Channel

Form of Error	Applicability		Estimated % Error						
	Thermal	Reflect.	Thermal		Reflectance				
			A	B	1.25	1.4	1.5	1.93	2.05
Analogue sample spectral measurement:	X	X	1.3	0.02	0.05	0.06	0.06	0.08	0.08
Mixing protocol errors		X	0	0	4.4	4.4	4.4	4.4	4.4
Greybody calibration target spectral characteristics	X	X	1.3	0.02	0.05	0.06	0.06	0.08	0.08
Borehole simulator spectral characteristics	X		1.3	0.02	0	0	0	0	0
Thermal channel emissivity optimization error.	X		1.12	3.19	0	0	0	0	0
Spectral confusion due to chemical bonds shifting absorption peak.		X	0	0	0	0	0	0	0
Removal of filters		X	0	0	2.0	2.0	2.0	2.0	2.0
Detector thermal stability	X		0.002	0.002	0	0	0	0	0
LED thermal stability		X	0	0	2.3	2.3	2.3	2.3	2.3
Filter thermal stability	X		0.002	0.002	0	0	0	0	0
Sample/calibration target thermal stability	X		0.005	0.005	0	0	0	0	0
Borehole simulator thermal stability	X		0.02	0.02	0	0	0	0	0
Filter spectral response range		X	0	0	0.05	0.06	0.06	0.08	0.08
Detector window spectral response range	X	X	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Electrical noise	X	X	1.0	1.0	1.0	1.0	1.0	1.0	1.0
LED spectral response range variability		X	0	0	1.0	1.0	1.0	1.0	1.0
Detector variability	X	X	0.05	0.05	0.05	0.05	0.05	0.05	0.05
Detector positioning	X	X	0	0	0	0	0	0	0
LED positioning	X	X	0	0	0	0	0	0	0
Instrument positioning in bore-hole		X	0	0	0	0	0	0	0
Measured System Error	X	X	0.08	0.08	2.5	2.5	2.5	2.5	2.5

	RMS Error:	6.1	6.1	6.1	6.1	6.1
Thermal RMS Error for Mini-TES sample P3004:	2.7	3.4				
Thermal RMS Error if pure, known sample:	2.5	1.1				
Thermal RMS Error if pure, unknown sample:	9.3	27.0				

The reflectance channels have an estimated system error of 6.1%. This was calculated as the same for all 5 channels because the largest sources of error were estimated as the same for all channels (Mixing protocol errors: 4.4%; Removal of Filters: 2.0%; LED thermal stability: 2.3%; and Measured System Error: 2.5%).

The two thermal channels had significant differences in the total system error. The narrow-band channel (Channel A) was calculated at 2.7%. The wide-band channel (Channel B) was calculated at 3.4%. These calculations used the bulk, undisturbed spectra from Mini-TES (Figure 4-3). If the samples are pure, the errors can be significantly larger. If the samples will be unknown, so that their spectral properties cannot be used to further refine the correlation to the surface temperature and the errors rise to 9.3% and 27% for channels A and B, respectively. If, on the other hand, some knowledge of the samples and their spectral properties are known, then the error in the two thermal channels can be reduced to 2.5 and 1.1%, respectively. The variation in emissivity for the 12 samples used in this thesis from the lowest to highest in comparison to the average for all 12 drives this calculation. In Channel B, the emissivity ranged from 0.47 to 0.90 with an average of 0.63, resulting in a maximum difference of 0.27. In Channel A, the difference was 0.09. This confirms the previous recommendations either to include a narrowband filter or to have knowledge of the materials being measured through other supporting instruments as discussed in Section 5.8.

6.11 Science and performance requirements update

The instrument performance traceability matrix (Table 3-8) was updated with the results of Chapter 6 in Table 6-10. All requirements were met in the measured performance, less the narrowband thermal IR channel, which was not constructed, and no measurements taken. This was left as not completed.

6.12 Conclusions and recommendations for future work

The measured reflectance was demonstrated to match the predicted result for a pure sample of CaCO_3 in all five channels with benchtop electronics. The custom design had limited performance with good results only in the 1.25 and 1.5 μm channels. The results in the other channels appear to have been limited by engineering choices that could be solved with additional expenditures as discussed in Section 7.4. A final set of recommendations for future development of this instrument are made here. This is in addition to any of the recommendations that were already adopted into this design or made in the previous chapters.

- Investigate the potential for a different detector/sensor
- Investigate the possibility for a different set of LEDs with higher power output or a new design in the 1.4, 1.95, and 2.05 μm channels
- Investigate the possibility for direct thermal control of the detector and LEDs with active heating and active cooling
- Include a dynamic gain circuit
- Improve the Phase Sensitive Detector circuit

These will be discussed in detail in the final chapter Summary, Conclusions, and Future Work, which will also consider this sensor design in context of Mars missions as well as other potential uses of this technology both on Earth and beyond.

Table 6-10: Science requirements to instrument performance traceability matrix (revised Table 3-8)

Science Objective	Observable Signatures	Measurement Goals	Spectral and Radiometric			Coverage and Sampling
			Channels	Performance Requirements	Measured Performance	Requirements and Performance
1. Determination of Water Ice and/or Bonded water	Absorption Peak at 1.93 μm of reflected light	>5% water content	1.5 μm	High reflectance band with accuracy $\pm 10\%$	$\pm 2.5\%$	Required: • 38° unobstructed FOV of surface • Spot size 17 mm dia. @ 11 mm from detector chip • Vertical resolution 17 mm • Integration time <30s. Performance: • 38° unobstructed FOV of surface • Spot size 17 mm dia. @ 11 mm from detector chip • Vertical resolution 17 mm • Integration time <60 s (max)
			1.93 μm	Absorption band with accuracy $\pm 10\%$	$\pm 2.5\%$	
			2.05 μm	High reflectance band with accuracy $\pm 10\%$	$\pm 2.5\%$	
2. Determination of Bonded OH ⁻	Absorption Peak at 1.4 μm of reflected light	Measurement of specific minerals: jarosite.	1.25 μm	High reflectance band with accuracy $\pm 10\%$	$\pm 2.5\%$	
			1.4 μm	Absorption band with accuracy $\pm 10\%$	$\pm 2.5\%$	
			1.5 μm	High reflectance band with accuracy $\pm 10\%$	$\pm 2.5\%$	
3. Determination of non-hydrated minerals	Flat spectral signature across water absorption peaks at 1.4 μm and 1.93 μm of reflected light	Measurement of specific minerals: basalt	Broadband IR Thermopile (0.4 μm to 50 μm), with 5 Channel LED sources	Thermopile IR wide passband 0.4 μm to 2.5 μm with >70% transmission; LED channels emitting at 1.25, 1.4, 1.5, 1.93, and 2.05 μm wavelengths.	Thermopile frequency response range 0.4 to 50 μm with >72% transmission. LEDs cover required bands.	
4. Determine temperature of subsurface environment	Emitted thermal flux	190-330 K $\pm$ 3 K	Broadband IR Thermopile (0.4 μm to 50 μm)	Thermopile IR passband with accuracy <3 K over 190-300 K range.	$\pm 0.2\text{K}$	
			Narrowband IR Thermopile (25.2 μm $\pm$ 30 nm)	Thermopile IR passband with accuracy <1 K over 190-300 K range.	Not Completed	
5. Determination of specific minerals found on Mars (Project Goal)	Shape and intensity of spectral curve across all channels of reflected light	Measurement of specific minerals: calcium carbonate, gypsum, jarosite, basalt	Broadband IR Thermopile (0.4 μm to 50 μm), with 5 Channel LED sources	Thermopile IR wide passband 0.4 μm to 2.5 μm with >70% transmission; LED channels emitting at 1.25, 1.4, 1.5, 1.93, and 2.05 μm wavelengths.	Thermopile frequency response range 0.4 to 50 μm with >72% transmission. LEDs cover required bands.	

Chapter 7: Summary, Conclusions, & Future Work

7.1 Overview and summary of Chapters 1 to 6

The hypothesis of this thesis that, *The subsurface environment of Mars provides habitable conditions sufficient to support life*, was defined at the beginning of Chapter 1. A series of questions to quantify the habitability of any location were proscribed in Table 1-1. These led to science objectives based on the expected environmental conditions on present day Mars and necessary conditions and materials to support the habitability as we understand it (Table 1-4). A review of previous missions to Mars provided some constraints to the proposed instrument for this thesis, in terms of size, power, and operations. The measurement of thermal infrared emission and infrared reflectance from the surface of a material was selected as the method for the determination of thermal and material properties. The remainder of the chapters were dedicated to the determination of appropriate analogue materials and environments necessary for the development of the thesis; identification and testing of individual components; development of IR thermal emission and reflectance models; and the development and testing of a technology demonstrator to show that an instrument concept could produce results that would match the predicted results from the integrated models. The science requirements (Table 1-4) were used to set the instrument performance requirements in Chapter 3 (Table 3-8) and updated in Chapter 6 (Table 6-12).

The integrated prototypes built and tested in Chapter 6 demonstrated that the science and performance requirements could be achieved; however, there were some limitations in the designs that could be improved in a future flight instrument. These are discussed for the thermal and reflectance channels in the following sections.

7.2 Thermal Channels A & B

Summary of experiments and results

Integrated system thermal models were developed for Channels A and B in Section 5.2. The performance for both channels predicted that they would have matching calibration curves (Figure 5-7 and 5-8) separated by voltage levels with the wideband Channel B predicted to generate significantly higher voltage levels.

Testing of these channels in the first prototype demonstrated that the thermal channels would be capable of measuring surface temperatures within the performance requirements (Figure 6-4). The principle error was lack of thermal control. Thermal control was added in the second prototype, Channel B, in a borehole configuration. The experimental design was modified to simulate a borehole environment. Results were linear (Figure 6-14) when tested with samples calibrated to a Nextel painted surface. Temperature errors ranged from 0.05 to 0.21 K (Table 6-4). The addition of thermal control designs and protocols allowed an instrument performance (D^*) of 1.55×10^9 and a Signal to Noise Ratio (SNR) of 3.3×10^7 .

The results of the testing of these prototypes showed that the performance of the instrument was well within the science requirements (Table 1-4) and performance requirements (Table 6-10) for both channels. These results were limited by the experimental setup to measure a flat sample, the calibration scheme, lack of an available 25.2 μm filter, and by the sensitivity of the detector.

Potential improvements to the experimental design and instrument

Experimental Design

The experimental design was limited by not having a simulated borehole within sample materials. This type of setup has been previously designed and built (Zacny et al., 2005, Zacny, 2004, Zacny, 2005). In this setup, a block of material was set inside a vacuum chamber that could be evacuated to Martian atmospheric pressures. A drill device was then activated to drill a borehole under Mars simulated pressures. This approach could be repeated with a larger thermal

vacuum chamber with a block of pre-drilled material. The instrument probe could be inserted into the borehole prior to closure or via a remote system. In this configuration, the only sources of radiance would be from the sample material in the FOV and reflected energy from sample material beyond the FOV of the detector and energy from the probe itself. This would more closely match an expected Mars mission scenario.

Instrument Calibration

The thermal calibration method used for this testing was with a flat aluminium surface that had been sandblasted and painted with Nextel black paint. In the best case, the emissivity of this would be 0.98. With degradation over time, it dropped to a measured 0.88. A further issue was that the surface was flat and not in a borehole configuration. This was accounted for in the calculations, but was not ideal.

Similar to a borehole simulator described above, the calibration should have the same form and diameter as the expected borehole to reduce radiances from sources other than the calibration target and the probe. This could be either a half-cylinder or a borehole cradle as shown in Figure 7-1. The instrument would be stored and calibrated in this cradle. This will allow more accurate modelling and accounting of radiances not attributed to the sample.

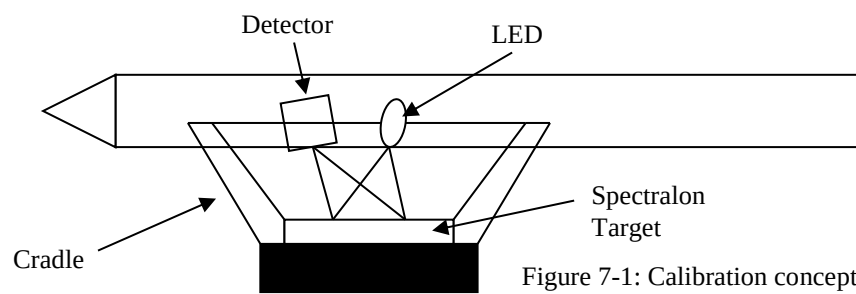


Figure 7-1: Calibration concept for field and Mars applications

Another potential improvement is to increase the emissivity of the calibration target. A recent technology developed in the UK in 2014 by Surrey NanoSystems is the Vantablack material (Harrington, 2016). This is an ultra-absorbent, black material made out of carbon nanotubes. The manufactures' datasheet claims an absorption coefficient of 99.9% from a prepared flat surface in the 700 nm to 3 μm range (Surrey-Nano-Systems, 2016). Of course,

degradation over time is still an issue, especially with dust storms on Mars, so a protective case would be needed to ensure that the surface was kept clean and free from particulates.

Narrowband Channel A

Testing of the borehole configuration (Thermal Prototype II in Section 6-4) was limited to the wideband Channel B because of a lack of an available 25.2 μm filter. This meant that the calibration shown in Figure 6-14 required prior knowledge of the emissivity of the tested samples. The original design to include a narrow band filter was because this allows the correct temperature measurement of an unknown surface without some prior knowledge of the material emissivity. An advantage to the configuration tested without the filter was that a single detector could be used for both the thermal and reflectance channels. If this filter was added, either a second detector would have to be added or a filter wheel that would have multiple filters including the 25.2 μm and reflectance channel filters.

Detector Sensitivity

The instrument performance, or effective D^* , is most directly affected by the thermal control of that detector and the sensitivity could be improved by using a better thermal control scheme than was implemented for this testing.

In this design, thermal control was maintained with a ceramic heater thermally coupled to the aluminium block. The external temperature was used as a heat sink to draw energy out of the system. This worked reasonably well in this system and improved the D^* a magnitude over the manufacturers measured result (Table 3-1 vs. Table 6-5). A better way to accomplish this; however, would be to include a two level Thermal Electric Cooler (TEC) control scheme that allows heating and cooling in order to keep a tighter temperature range. Keeping with the multi-layer concept as tested, the first level of control would be to change the ceramic heater on the aluminium block to a TEC. This would allow the temperature range of the entire detector to be more tightly controlled. The second level would be to switch to a detector that has a TEC built directly into the can to allow direct control of the chip temperature. This design is used in the LEDs produced by IBSG (the 1.95 and 2.05 μm channels) to stabilize the temperature of the LED chips to prevent drift in the spectral output. This same packaging and approach could be used for

the thermopile chip to be substituted in for the LED chip on the TEC stack in Figure 7-2 (IBSG, 2012) .

One issue that results in the two-level temperature control scheme is that the can and filter temperature could have a different temperature than the detector chip itself, resulting in a radiance term that is not related to the scene. This would have to be

carefully considered either to take data when the temperature of all the detector components are the same or to account for the additional radiance terms in the calculations.

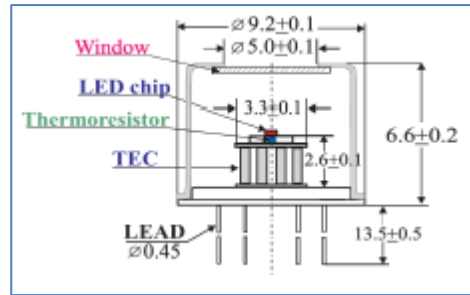


Figure 7-2: ISBG thermally controlled LED with diode mounted on a TEC stack

7.3 Reflectance Channels: 5 bands

Summary of experiments and results

Integrated system reflectance models were developed for Channels 1 to 5 in Section 5.4. The predicted performance of all channels resulted in matching the mineral reflectance characteristics (Figures 5-12 and Appendix Figures A-1 to A-4), with some spectral confusion errors noted in Table 5-4. A channel ratio analysis of water ice and hydrated minerals mixed with non-hydrated minerals determined that several combinations of channels could be used to detect and discriminate water ice, hydrated minerals, and their concentrations within a non-hydrated matrix (Figures 5-21 to 5-24).

Based on the assumption of a pulsed LED at full power, the 1.93 μm channel was calculated to have enough energy to perform the required task with an SNR of at least 1260 for Saponite (Section 5.4 and Appendix Table B-4). It was also noted that this channel had the most error because of the spectral shapes for water ice and gypsum across this band and that a filter was recommended to reduce the spectral error (Table 6-8). This was not possible to test in the integrated instrument, as a filter was not available.

A bore-hole configuration of the reflectance channels (Figure 6-28) was tested with benchtop electronics and pure minerals and was found to measure the reflectance in all channels

within expected tolerances (Figures 6-36 to 6-40). A repeat of the test with the custom electronics was only able to work with the high power 1.25 μm and 1.5 μm LEDs (Figures 6-43 and 6-44). These results were limited by additional radiances due to the calibration methods, the selected channel positions, the forward optical power of the LEDs, detector sensitivity, and the custom electronics. Additional issues were the lack of dedicated channel filters and the LED spectral variability associated with LED temperature fluctuations.

Potential improvements to the experimental design and instrument

Updated calibration scheme

Like the thermal channels, the accuracy of the results is dependent upon a good method of regular calibration of the voltages generated by the detector when tested with sample materials. The final version of the experiment relied on flat calibration targets for a highly reflective material: Spectralon with well-characterized reflectance properties and a Nextel painted greybody with a low reflectance. Similar to the recommendations for the calibration of the thermal channels, the two calibration materials should be formed in a borehole like cradle. The Vantablack material is also recommended for the two-point calibration of the reflectance channels.

Channel position selection

The original selection of channels was by review of the literature to determine appropriate absorption features for water ice and hydrated minerals. This identified the 1.45 μm and 1.93 μm as key absorption features for hydroxide and water, respectively. The other 3 channels were selected primarily as anchor bands. All five channels were limited to commercially available LEDs and filters. Solutions were found for the key absorption features while the others were selected by what was available. The results of testing determined that the absorption channels and the 1.25 μm as a reflectance channel were central to the functionality of the device. The 1.5 μm had limited use, while the 2.05 μm channel may not even be necessary. Similar to what was done for the PanCam on ExoMars (Cousins et al., 2010), there is an opportunity to optimize the channel positions for this instrument. This would require a principal components analysis (PCA) of all of the expected minerals, pure and mixed spectra, to determine what would be the optimal spectral

positions for the 5 bands. For a flight instrument, this analysis is highly recommended and would lead to custom filters; however, the final positions may still be limited by commercially available LEDs to match these new channel positions.

Forward optical power of the LEDs

The forward optical power of the LEDs is one of the two most important characteristics to make this a functional system (with the detector sensitivity as the second). The LEDs manufactured by Thorlabs (1.25 and 1.5 μm channels) had significantly higher forward optical power than the other three. Increasing the forward optical power to provide more reflected energy is necessary. There are three options for improving this: 1) increasing the current supply to the LEDs to increase the forward optical power of the existing LEDs, 2) selection of a different manufacturer with a higher forward optical power parameter, and 3) increase the number of LED chips for each channel.

Increasing current supply:

This was implemented in this project. The early models utilized the maximum forward optical power assuming a pulsed current supply with a 1% duty cycle. The maximum allowable current to the ISBG LEDs (1.95 and 2.05 μm) per the manufacturers' data sheet was not reached during testing, even with a 2% duty cycle. This is because the lead product engineer for the UK distributor of that component recommended that a maximum supply voltage of 2.5 VDC not be exceeded (verbal communication: Demetri Permogorov, IBSG/Deep Red Technologies, Harwell, UK, 08/07/2015). The results with the custom electronics were below the detectivity threshold of the circuit. Because it was shown that these three channels could be detected with the benchtop electronics, improvements to the forward optical power by a better current supply to the LEDs would help the performance of the integrated system.

Alternative LED manufacturer

Substitution of an LED with a higher forward optical power is another way to increase the forward optical power; however, there are not many manufacturers of compact IR LEDs, so options are limited. For the 1.4 μm channel, it appears that Thorlabs has added an LED (P/N: LED1450-L) with the same exact packaging as the one from Hamamatsu. The technical

datasheet notes that it has a forward optical power about twice that of the Hamamatsu. However, it looks identical to the Hamamatsu LED, and very well could be produced by the same third-party company with the differences in technical performance attributed to different internal test procedures implemented at Thorlabs and Hamamatsu. For the 1.95 and 2.05 μm channels; however, an alternative manufacturer with the small package size has yet to be identified.

Multiple chip LED design

The most complicated and expensive solution would be to create a single LED package with multiple chips. Presumably, 2 LED chips would double the forward optical power. In discussions with Deep Red Technologies (Verbal communication, D. Permogorov, Deep Red Technologies, Harwell, UK), it was indicated that there are custom options available to place up to 9 LED chips into a single small can design. This is actually quite interesting as an option to improve the forward optical power. This could both improve the forward optical power of the individual channels as well as improve the geometry of the instrument. The best alignment of LED and detector would be when they are placed inline at a 45° angle to the surface. This was not possible in the current design because of the use of individual LEDs placed in a cluster around a single element detector. With a 9-chip package, it would be possible to include three each of the 1.95 μm and 2.05 μm LEDs from ISBG, one 1.45 μm LED from Thorlabs (assuming it does have double the optical power as compared to the Hamamatsu), and one each of the 1.25 μm and 1.5 μm LED chips from Thorlabs. This should be combined with the in-can TEU design shown in Figure 7-1 to control the temperature and spectral output peaks.

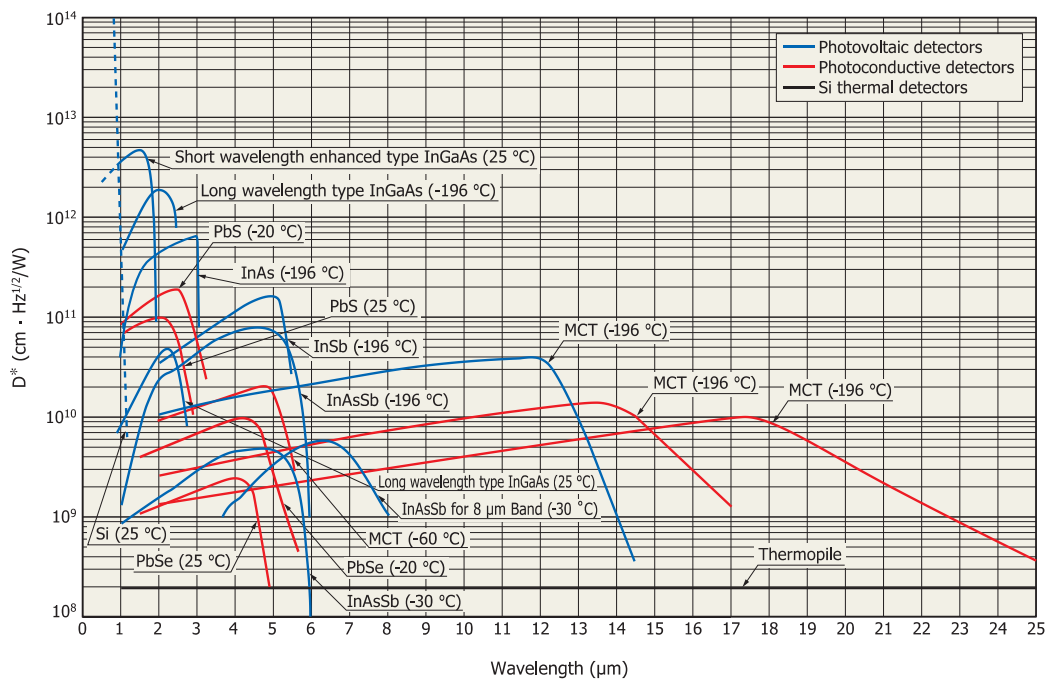
Detector Sensitivity

The thermopile solution utilized in this thesis (Section 3.3) was selected because of the space heritage of thermopiles and because the original calculations indicated that it should be sensitive enough to measure both the thermal IR emission and IR reflectance.

The thermopile D^* can be improved for measurement in the thermal channels by controlling the temperature, but there was no way to improve the D^* for the reflectance channels. In the reflectance channels, the detector performance, detectivity or D^* , is dependent upon the substrate of the chip material. A different detector for the reflectance channels would be required

to improve the detector performance. The thermopile has a flat performance across the entire response range out to 25 μm (assuming no thermal control) with a $D^* = \sim 10^8$. The thermopile performed adequately as tested in this thesis; however, improvements to the D^* in the reflectance channels is desired. There are a number of options that could satisfy this need as shown in Figure 7-3 (Hamamatsu Detector Catalogue). The two best options would be a short wavelength enhanced type InGaAs photovoltaic detector operated at 25°C or a PbS photoconductive detector operated at -20°C. The InGaAs detector has a D^* in the $10^{12} - 10^{12.5}$ range, but the spectral response drops rapidly above 1.6 μm and might not have enough range to capture the 1.95 μm signal. The PbS has a wider response range of 1-3 μm , but has a lower D^* at 10^{11} . Both should be tested, as these would provide 3 to 4 magnitudes better performance than the thermopile. These should be combined with the in-can TEU design shown in Figure 7-1 to control the temperature.

Figure 7-3: Hamamatsu Detectors Spectral Response Range



Custom electronics performance

The system was shown to work with the benchtop electronics, but failed to work with the custom electronics in the 1.4, 1.95, and 2.05 μm . The assumption of pulsed current to the other LEDs resulted in calculations that indicated that the single gain value would be sufficient to detect and discriminate materials in all channels (Section 5.3 and Appendix Table B-4). In practice, this

was not the result when the supply current was significantly limited in these channels. While recommendations have been made to improve both the current supply and the detectivity in these channels, one immediate recommendation for the custom electronics is to design in dynamic gain to increase the range of amplification options. The other recommended change would be to update the phase adjustment to an automatic digital design. In this design, a 10 k Ω potentiometer was used to tune the phase adjustment (aligns the read command to the peak of the incoming pulsed signal), but this would be significantly improved with a dual channel lock-in with a digital phase adjustment.

Individual channel filters

The results of testing showed that the science requirements could be met without filters (Table 6-8, Section 6.6); however, spectral confusion can be reduced with the use of filters and is desirable in the design of a flight instrument. This is going to have to be balanced with the other design choices. A single LED package will make this difficult unless the filters could be mounted inside the can over each individual element. If, on the other hand, the current cluster design is utilized, then filters could be designed and built to be placed over each of the LEDs. Filters will reduce the amount of reflected energy to about 1% of the current values, so a higher performing detector would have to be selected to go with any solution using filters. An additional step would be to have better matching of the LED and filters. Figures 3-23 to 3-27 matched these, but the 1.25 μm and 1.5 μm channels could be better. Table 6-8 calculated the errors associated with removing the filters, attributing an estimated 2% error. Improved filter matching would eliminate this type of error.

LED spectral variability

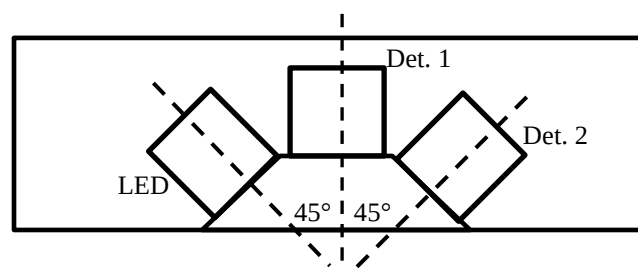
The LED spectral peak varies with temperature as shown in Figure 5-27. In the current design, the thermal stability of the LEDs were controlled by mounting them into the temperature controlled aluminium block. The ideal peak; however, will be different for each individual LED. The preferred design solution would be to have each LED chip individually thermally stabilized. This can be accomplished as was shown for the IBSG LEDs in Figure 7-1. This solution is currently only available for the IBSG LEDs; however, collaboration with the different

manufacturers could produce individual LEDs with this packaging as well as the multi-chip LED version that could include the TEC stack as part of the design. These solutions would allow tightly controlled peak frequencies for each of the individual channels and would reduce the spectral confusion error. Barring the potential for a new LED design solution, the LED spectral distribution could be measured as a function of temperature so that the models would at least allow a correction to the calibrated value as long as the temperature of the individual LEDs are recorded at the time of the measurement. This temperature control of the LED spectral output would also help in the matching with the filter transmission characteristics.

7.4 Improved Instrument Concept

The original instrument concept (Figure 1-5) was followed throughout the development of this thesis, leading to a prototype (Figure 6-28) which included many of the original design concepts as well as modifications as the advantages and limitations of each component were discovered, considered, and integrated into the final design. Testing provided additional lessons learned and identified potential modifications for a flight instrument. One potential layout for this improved instrument concept is shown in Figure 7-4. In this concept, there are two detectors and one multi-element LED chip package as the source. These are set into an aluminium thermal block inline along the length of the device. The thermopile detector (the Dexter S25 with a 25.2 μm window) is positioned to look directly at the surface (Det. 1). The multi-chip LED package and InGaAs or PbS detector (Det. 2) for the reflectance channels are oriented at a 45° angle to the surface directly opposite to each other in order to maximize the energy reaching the detector by setting the angle of reflectance equal to the angle of incidence. Both the LED and Detectors are recommended to include the in-can TEU design (Figure 7-1) to control the temperature at the chip.

Figure 7-4: updated geometry for next generation of the Mars borehole instrument



This update to the design is anticipated to significantly improve the instrument performance by designing and building new components that maximize the individual component performance while placing them into a geometry that optimizes the energy reaching the detectors in both channels. Switching to the InGaAs or PbS sensor in the reflectance channels alone would be a significant improvement, but when combined with a better LED design, improved instrument component geometry, and improved electronics, most of the limitations encountered during the thesis project would be eliminated.

A limitation to this concept is that no individual channel filters are included, leading to the same spectral confusion errors encountered in the prototype utilized in this thesis (Figure 6-28). Two options for this could be the addition of a filter wheel/feeder or placing filters directly over the LED chips within the multi-element LED package.

7.5 Expected outcomes during a Mars mission

This thesis developed an instrument to satisfy the science objectives listed in Table 1-4. Now the question is, how well did it do? This will be considered in the context of the as designed instrument and in terms of the updated design presented in Section 7.4.

Temperature measurement

The requirement listed in Table 1-4 was for a range of 190-320 K with an allowable error of <1 K (Channel A) and <3 K (Channel B). With Channel B testing, there was a measured error of ± 0.2 K (or $\sim 0.08\%$). This result was well within the requirements of <3 K. The key limitation was the missing Channel A 25.2 μm filter. Table 6-9 calculated the errors associated with measurement of a pure, unknown mineral. Channel A would be as much as 9% while Channel B would be as much as 27%. These would push the performance beyond the <1% and <3% temperature errors allowed for Channels A and B, respectively. This would be the worst-case, as it is anticipated that knowledge of the emissivity from the reflectance channels and other instrumentation (Section 5.8) would reduce these errors.

Water ice: detection and discrimination

The detection of water ice and the discrimination of the concentration in a soil matrix was demonstrated by a model developed in Chapter 5. The original requirement was for positive/negative detection and for a discrimination range of 1-15% (Table 1.4), though this was modified to >5% concentration with an allowable error of $\pm 10\%$ (Table 3-8). The model tested the different combinations of channel ratios for water ice mixed with Pyroxenes (Figure 5-21) and Palagonite (Figure 5-22). The 1.25 μm – 1.93 μm channel ratio was the best result for the water ice models.

In these figures, it was shown that the capability to detect water ice was accomplished with a detection limit $1 \pm 1\%$. This matches the requirement established in Table 3-8. The discrimination of water ice shown to be possible from 5% to 60% with an error of $\pm 1\%$ concentration in both mineral matrices. Water ice saturates the signal in the 1.93 μm channel quickly, relying on the 1.25 μm water ice reflectance feature to provide the discrimination capability. This met the requirement for a range of at least 1-15% with an error of $\pm 10\%$.

The original intent was to test in Mars analogue environments, but travel funds for testing in University Valley, Antarctica, were eliminated from the budget during the project. Due to lack of travel funds and a thermal vacuum simulation chamber capable of handling water ice at Mars temperatures; measurement of water ice under Mars simulated or analogue conditions remains untested.

The results of a much lower than expected energy in the 1.93 μm channel suggest that satisfaction of these requirements could be at risk if this thesis design is implemented. Since detection and discrimination of water ice is the most important requirement, and because the 1.93 μm channel is critical to the satisfaction of this requirement, an update to the flight instrument to increase the 1.93 μm LED forward optical power and the detector sensitivity is essential.

Hydrated minerals: detection and discrimination

The detection of hydrated minerals and the discrimination of the concentration in a soil matrix was demonstrated by testing in Chapter 6. The original requirement was for the positive/negative detection (Table 1-4) using the absorption features at 1.4 μm and 1.93 μm for hydroxide and water, respectively (Table 3-8). A percent discrimination was not defined beyond an instrument performance of $\pm 10\%$ in each channel. The models in Chapter 4 determined which ratios were most effective to satisfy these requirements with mixed materials and the integrated models in Chapter 5 were compared with testing of mixed minerals. The results were provided in Figures 5-23 (1.93 μm) and 5-24 (1.4 μm) for gypsum mixed with pyroxene, and in Figures 5-25 (1.4 μm) and 5-26 (1.93 μm) for montmorillonite mixed with palagonite. Both mixtures and combinations showed that positive detection was possible, but that the concentrations of the hydrated minerals had to be at least $>25\%$. Testing with pure minerals in Chapter 6 (Figures 6-36 to 6-40) determined the error to be about 2.5% in all channels. This met the terms of the original requirements, but the lack of low-end concentration resolution is a significant disadvantage. Both of these ratios rely on two of the weakest LEDs, so low-end resolution will be challenging if the thesis solution is implemented and if the discrimination of low-end concentrations is a requirement. The updated solution with higher forward optical power and detector sensitivity will be essential for a flight instrument. This would increase the low-end detection and push the discrimination to a much lower concentration.

7.6 Beyond Red Planet Mars

This thesis was tied to Mars because of the NASA funding associated with the IceBite project. Mars, from an Astrobiology perspective, is interesting as a destination with lots of questions to pose and answer, and this instrument could be integrated into many mission scenarios including moles, landers, rovers, fixed wing planes, balloons, and entry vehicles (to name a few). However, Mars is not the only interesting destination in the solar system. Here I discuss a few opportunities.

Le Voyage dans La Lune (A trip to the Moon)

The Moon is the most obvious choice for an alternative destination for this technology. *In situ* resource utilization would significantly reduce the cost of long-term lunar missions. Finding large quantities of accessible water ice on the surface is important because it can be used as a source of potable water as well as an oxidizer for rocket propellant. Finding water as part of *in situ* resource utilization is a major goal for the space agencies and is even a \$5 million bonus prize for the Google Lunar XPrize. In addition to water, organic materials deposited by comets, ^3He which is an important component for fusion reactors, and base materials (e.g., olivines or pyroxenes) for construction of lunar bases and landing fields would all be important to be able to cheaply and accurately identify. While the water channels were already determined in this thesis, the other materials will have their own spectral absorption features. As long as these features are within about 400-2500 nm wavelengths, both filters and LEDs could be selected to allow the detection and discrimination of these materials.

MacNab Visits the Comet

Comets and asteroids are the next alternative destination. Much like the Moon, these either are made principally of water ice (comets) or have accumulated water ice over time. These also have a certain amount of organic materials and other minerals, all of which can be used for *in situ* resource utilization. Another emerging field is asteroid mining in the search for high value minerals such as nickel and titanium. Companies such as Planetary Resources are already searching for high value asteroids, and a way to identify the minerals they are looking for, as part of a surface lander is highly desirable.

Планета Бур (Planeta Bur)

Venus is another potential destination, but not as part of a surface lander. The surface of Venus is highly acidic and hot. This technology would probably not work. One of the current concepts for Venus is the use of a balloon type UAV. In this case, a highly compact, low-weight and power, filter radiometer could be built utilizing many of the components of this instrument.

LEDs would no longer be necessary as reflected sunlight would provide the energy source. Single or multi-element thermopiles with filters placed in front of them or with a filter wheel would provide a very nice solution for the measurement and characterization of the Venus atmosphere.

The Day the Earth Stood Still

Earth is the last and best example of a potential destination. There are many exciting opportunities for the use of this technology in Earth based applications. As part of the balloon concept, it could be used to measure atmospheric properties. It could have a strong case in the mining industry for the identification of sub-surface minerals. Because it is compact and low cost, there are hundreds of applications in the developing world as an alternative to expensive spectrometers.

7.7 Conclusions

The motivation for this thesis was for the creation of a new instrument that could be used to aid in the search for life in the sub-surface of Mars. In particular, the original NASA IceBite proposal, which funded this thesis, was to design an instrument that would characterize the concentration of water ice in a soil matrix. This was expanded to include hydrated minerals and temperature of the materials. An instrument was designed and tested that was shown to have the capability to detect and discriminate materials and to measure the temperature of known materials. While the results were successful, some limitations were identified and recommendations were made for flight instrumentation that could be sent To Mars and Beyond.

- The End -

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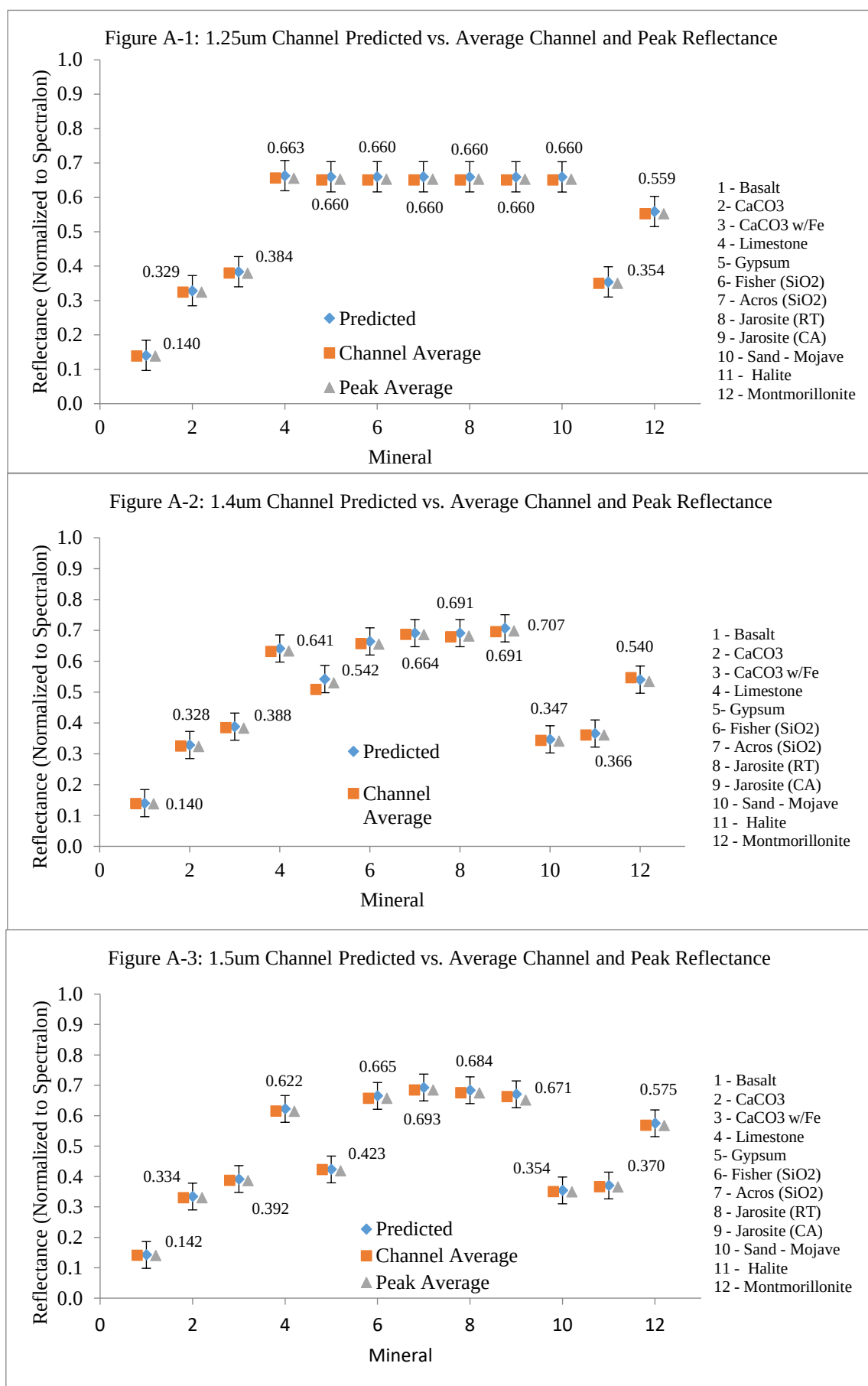
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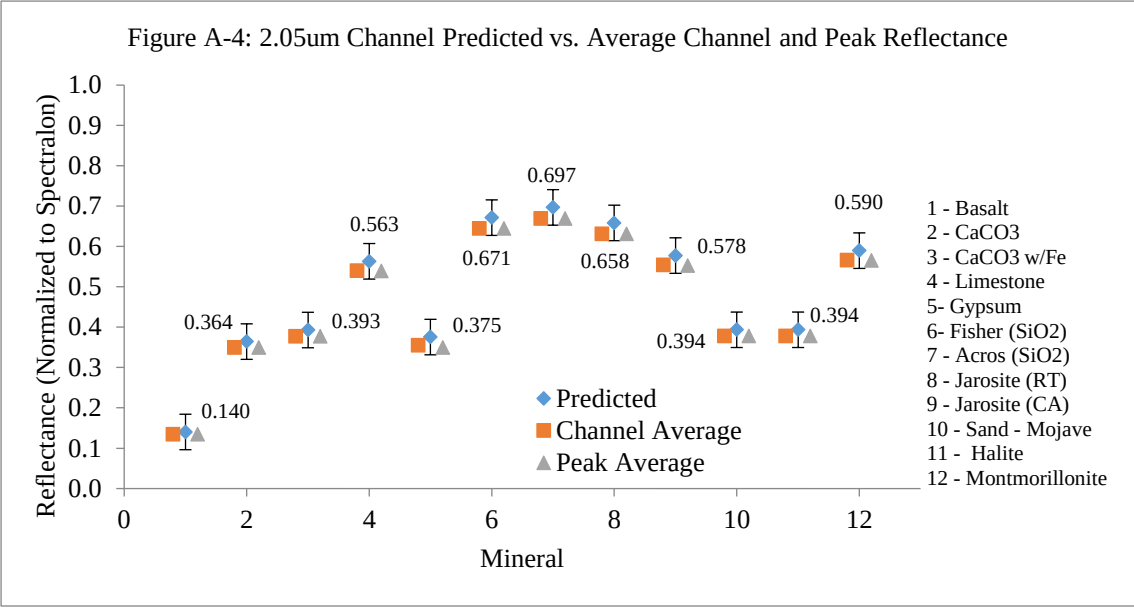
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Appendices

Appendix A: Additional Figures



Appendix A: Additional Figures



Appendix B: Additional Tables

Table B-1: Channel A (Narrowband) Radiated Energy

	150	160	170	180	190	200	210	220	230	240	250	260	270	280	290	300
Basalt	0.2499	0.3306	0.3958	0.4804	0.5747	0.6703	0.7746	0.8846	0.9997	1.1196	1.2439	1.3723	1.5044	1.6399	1.7786	1.9203
CaCO ₃	0.2592	0.3430	0.4105	0.4983	0.5961	0.6953	0.8036	0.9177	1.0371	1.1615	1.2905	1.4237	1.5608	1.7014	1.8454	1.9924
CaCO ₃ _Fe	0.2587	0.3424	0.4098	0.4974	0.5951	0.6941	0.8021	0.9160	1.0353	1.1595	1.2882	1.4212	1.5580	1.6983	1.8420	1.9887
Limestone	0.2278	0.3017	0.3611	0.4384	0.5248	0.6120	0.7074	0.8080	0.9134	1.0231	1.1368	1.2543	1.3752	1.4992	1.6262	1.7559
Gypsum	0.2595	0.3433	0.4110	0.4988	0.5967	0.6960	0.8043	0.9185	1.0380	1.1626	1.2916	1.4249	1.5621	1.7029	1.8469	1.9940
Jarosite_RT	0.2584	0.3419	0.4092	0.4967	0.5942	0.6931	0.8009	0.9146	1.0337	1.1577	1.2863	1.4190	1.5556	1.6957	1.8392	1.9857
Jarosite_CA	0.2555	0.3380	0.4046	0.4911	0.5875	0.6852	0.7919	0.9043	1.0220	1.1446	1.2717	1.4029	1.5380	1.6765	1.8184	1.9632
Sand_Mojave	0.2541	0.3362	0.4024	0.4884	0.5843	0.6815	0.7876	0.8993	1.0164	1.1383	1.2647	1.3952	1.5294	1.6672	1.8082	1.9522
Halite	0.2541	0.3362	0.4024	0.4884	0.5843	0.6815	0.7876	0.8993	1.0164	1.1383	1.2647	1.3952	1.5294	1.6672	1.8082	1.9522
Montmorillo- nite	0.2515	0.3328	0.3983	0.4834	0.5784	0.6746	0.7796	0.8902	1.0061	1.1268	1.2519	1.3811	1.5141	1.6505	1.7901	1.9327
Fisher_SiO ₂	0.2247	0.2975	0.3561	0.4323	0.5175	0.6035	0.6976	0.7968	0.9006	1.0088	1.1209	1.2367	1.3559	1.4782	1.6034	1.7312
Acros_SiO ₂	0.2195	0.2907	0.3480	0.4225	0.5057	0.5898	0.6818	0.7787	0.8802	0.9860	1.0956	1.2088	1.3254	1.4449	1.5673	1.6923
Average:	0.2477	0.3279	0.3924	0.4763	0.5699	0.6647	0.7683	0.8773	0.9916	1.1106	1.2339	1.3613	1.4924	1.6268	1.7645	1.9051
StDev:	0.0147	0.0194	0.0232	0.0281	0.0335	0.0391	0.0451	0.0515	0.0581	0.0650	0.0722	0.0796	0.0871	0.0949	0.1029	0.1110
100% Emissivity	0.2654	0.3386	0.4203	0.5102	0.6075	0.7119	0.8227	0.9395	1.0618	1.1891	1.3212	1.4575	1.5978	1.7418	1.8891	2.0396

Appendix B: Additional Tables

Table B-2: Channel B (Wideband) Radiated Energy

	150	160	170	180	190	200	210	220	230	240	250	260	270	280	290	300
Basalt	3.971	5.465	7.329	9.613	12.373	15.664	19.544	24.075	29.319	35.338	42.197	49.960	58.690	68.452	79.306	91.314
CaCO ₃	4.050	5.568	7.459	9.772	12.559	15.876	19.780	24.329	29.583	35.601	42.447	50.181	58.865	68.559	79.322	91.212
CaCO ₃ _Fe	4.053	5.570	7.459	9.769	12.553	15.865	19.762	24.301	29.542	35.545	42.371	50.080	58.734	68.392	79.112	90.951
Limestone	3.731	5.161	6.948	9.142	11.794	14.957	18.687	23.040	28.073	33.844	40.414	47.842	56.185	65.502	75.849	87.283
Gypsum	4.068	5.591	7.486	9.805	12.601	15.930	19.848	24.416	29.695	35.745	42.629	50.410	59.149	68.908	79.747	91.723
Jarosite_RT	4.092	5.626	7.536	9.874	12.691	16.043	19.985	24.575	29.871	35.930	42.813	50.576	59.278	68.973	79.716	91.560
Jarosite_CA	4.040	5.555	7.443	9.755	12.544	15.865	19.777	24.338	29.610	35.652	42.528	50.298	59.024	68.766	79.583	91.531
Sand_Mojave	3.804	5.195	6.914	9.004	11.507	14.470	17.939	21.962	26.588	31.865	37.844	44.574	52.103	60.480	69.751	79.962
Halite	3.804	5.195	6.914	9.004	11.507	14.470	17.939	21.962	26.588	31.865	37.844	44.574	52.103	60.480	69.751	79.962
Montmorillo- nite	3.992	5.492	7.361	9.651	12.414	15.706	19.582	24.103	29.328	35.317	42.130	49.830	58.475	68.125	78.837	90.667
Fisher_SiO ₂	3.511	4.839	6.495	8.525	10.975	13.893	17.328	21.334	25.963	31.270	37.311	44.144	51.825	60.413	69.963	80.533
Acros_SiO ₂	3.409	4.700	6.311	8.287	10.671	13.511	16.855	20.755	25.262	30.430	36.314	42.970	50.454	58.823	68.132	78.438
Average:	3.877	5.330	7.138	9.350	12.016	15.187	18.919	23.266	28.285	34.034	40.570	47.953	56.240	65.489	75.756	87.095
StDev:	0.229	0.312	0.415	0.544	0.701	0.891	1.119	1.389	1.706	2.074	2.497	2.979	3.526	4.140	4.825	5.586
100% Emissivity	4.182	5.750	7.703	10.096	12.982	16.422	20.474	25.203	30.671	36.945	44.090	52.173	61.260	71.415	82.704	95.188

Appendix B: Additional Tables

Table B-3: Integrated Channel Power for each Mineral

Mineral	Power Generated in Each Channel (nW)				
	1.25 μm	1.4 μm	1.5 μm	1.93 μm	2.05 μm
100% Spectralon	2038.9	357040.0	2202.0	519.7	102250.0
Albite	1749.2	311982.8	1931.7	452.8	92566.3
Anhydrite	1847.1	324931.6	2004.2	450.7	94471.0
Augite	318.9	69869.1	484.5	171.8	37652.3
Calcite	1766.0	312016.8	1919.8	443.6	89538.2
Chromite	261.2	48660.3	251.0	35.4	6627.3
Hematite	714.3	125901.9	777.4	194.8	40255.3
Ilmenite	123.8	22372.2	138.9	33.8	6814.6
Labradorite	536.5	91840.3	561.0	136.1	28268.2
Maghemite	525.8	91293.9	552.2	140.7	30738.5
Magnetite	98.2	19772.1	133.3	39.5	8478.1
Olivine	276.3	82128.7	805.4	334.8	67873.0
Pyroxene	181.2	40866.5	302.5	127.5	29862.9
Quartz	1734.1	308778.0	1914.3	458.0	92538.1
Alunite	1716.7	302236.5	1581.0	403.5	72776.6
Analcime	1800.9	242139.8	1744.7	187.7	76270.2
Bassanite	1836.9	270204.9	1737.8	181.8	72290.7
Chlorite	646.0	134606.5	984.6	320.1	67868.8
Coquimbite	1454.7	228790.2	919.8	128.4	20086.5
epsomite	1099.6	104498.0	287.9	14.3	4718.4
Ferrihydrite	738.5	185660.1	1240.8	206.5	47626.3
Geothite	651.7	127691.0	799.0	182.1	38131.6
Gypsum	1709.8	269486.7	1377.5	165.5	62432.6
Halloysite	1687.4	190354.3	1641.0	256.7	62078.1
Illite	1294.6	178984.8	1350.2	266.9	58341.1
Jarosite	1155.1	267794.8	1610.1	410.0	74628.5
Kaolinite	1815.9	230347.9	1971.2	397.8	80825.2
Kierserite	1269.9	196342.6	664.0	92.2	10018.5
Montmorillonite	1572.6	251197.1	1227.3	309.8	40135.5
Muscovite	1478.0	214138.7	1738.7	394.7	80224.8
Nontronite	1061.2	159440.8	1065.2	154.3	45198.3
Opal	553.6	24929.3	174.3	14.0	4157.9
Prehnite	1316.5	220255.0	1088.8	251.9	54744.9
Saponite	1680.2	161291.1	1332.1	126.4	45806.8
Serpentine	315.0	36175.2	347.1	64.3	13380.5
NEP	0.1	0.1	0.1	0.1	0.1

Appendix B: Additional Tables

Table B-4: Channel SNR for each Mineral

Mineral	SNR in Each Channel (nW)				
	1.25 μm	1.4 μm	1.5 μm	1.93 μm	2.05 μm
Albite	17492.4	3119828.4	19317.4	4528.1	925663.4
Anhydrite	18470.9	3249315.9	20041.9	4507.5	944709.7
Augite	3188.7	698690.5	4845.1	1718.4	376523.4
Calcite	17660.0	3120167.9	19198.4	4436.2	895382.3
Chromite	2612.2	486603.3	2509.8	354.4	66272.6
Hematite	7142.6	1259019.2	7773.6	1948.4	402552.7
Ilmenite	1237.6	223722.5	1389.3	338.1	68145.7
Labradorite	5364.8	918402.8	5610.2	1361.4	282681.8
Maghemite	5258.5	912938.8	5521.9	1407.4	307384.6
Magnetite	981.6	197721.3	1332.8	394.8	84781.2
Olivine	2762.5	821287.3	8053.9	3348.5	678729.8
Pyroxene	1812.3	408664.9	3025.4	1274.7	298629.3
Quartz	17341.3	3087779.8	19143.1	4580.3	925380.7
Alunite	17167.1	3022365.1	15809.6	4034.7	727765.8
Analcime	18008.8	2421397.7	17447.4	1876.5	762701.5
Bassanite	18369.4	2702048.8	17378.4	1817.5	722906.6
Chlorite	6460.2	1346065.4	9846.5	3201.2	678688.4
Coquimbite	14547.3	2287902.1	9198.2	1284.5	200865.4
epsomite	10995.8	1044980.2	2879.4	143.1	47184.2
Ferrihydrite	7385.0	1856601.4	12408.1	2065.2	476263.0
Geothite	6517.0	1276909.5	7989.9	1820.5	381315.6
Gypsum	17097.8	2694866.7	13774.7	1654.8	624326.3
Halloysite	16874.0	1903542.6	16410.4	2567.1	620781.4
Illite	12946.4	1789847.5	13502.2	2668.8	583411.2
Jarosite	11551.2	2677948.4	16101.3	4100.3	746285.0
Kaolinite	18159.2	2303479.2	19711.9	3978.3	808251.8
Kierserite	12698.5	1963426.0	6639.6	922.0	100184.8
Montmorillonite	15726.3	2511971.2	12273.3	3097.9	401354.7
Muscovite	14779.8	2141386.7	17386.9	3946.8	802247.6
Nontronite	10611.6	1594408.0	10651.9	1542.9	451982.9
Opal	5535.7	249293.3	1743.3	140.5	41579.3
Prehnite	13164.6	2202550.1	10887.8	2518.5	547448.9
Saponite	16801.8	1612910.9	13320.8	1263.7	458067.7
Serpentine	3150.2	361751.6	3471.5	642.7	133804.7

Maximum SNR:	1.8E+04	3.2E+06	2.0E+04	4.6E+03	9.4E+05
Minimum SNR:	981.6	2.0E+05	1332.8	140.5	4.2E+04

Appendix B: Additional Tables

Table B-5: Integrated Power Calculations for Mixed Water Ice with Pyroxene

Material mixture	Power Generated in Each Channel (nW)				
	1.25 μm	1.4 μm	1.5 μm	1.93 μm	2.05 μm
100% Reflection	2037.6	361780.0	2228.8	531.1	106420.0
100% Spectralon	2015.2	357040.0	2202.0	519.7	102250.0
100% Pyroxene	541.4	113300.0	750.4	168.9	30721.0
Pyr 99: WI 01	554.0	115420.0	726.3	163.7	29802.0
Pyr 95: WI 05	602.5	122920.0	649.4	147.0	26827.0
Pyr 90: WI 10	659.5	131520.0	582.7	132.4	24175.0
Pyr 80: WI 20	764.6	147180.0	499.0	113.8	20784.0
Pyr 70: WI 30	860.9	161060.0	448.3	102.4	18692.0
Pyr 60: WI 40	951.3	173540.0	414.3	94.8	17277.0
Pyr 50: WI 50	1038.8	184820.0	389.9	89.3	16254.0
Pyr 40: WI 60	1122.1	195240.0	371.4	85.1	15480.0
Pyr 30: WI 70	1205.1	204980.0	357.1	81.8	14874.0
Pyr 20: WI 80	1287.9	214140.0	345.5	79.2	14387.0
Pyr 10: WI 90	1372.1	222830.0	336.0	77.1	13986.0
Pyr 05: WI 95	1415.1	227030.0	331.9	76.2	13811.0
Pyr 01: WI 99	1450.3	230330.0	328.9	75.5	13682.0
100% Water Ice	1459.2	231140.0	328.1	75.3	13651.0
NEP	0.1	0.1	0.1	0.1	0.1

Table B-6: SNR Calculations for Mixed Water Ice with Pyroxene

Material mixture	SNR in each channel				
	1.25 μm	1.4 μm	1.5 μm	1.93 μm	2.05 μm
100% Reflection	20376.0	3617800.0	22288.0	5311.3	1064200.0
100% Spectralon	20152.0	3570400.0	22020.0	5196.5	1022500.0
100% Pyroxene	5413.8	1133000.0	7504.4	1688.6	307210.0
Pyr 99: WI 01	5539.7	1154200.0	7262.7	1636.8	298020.0
Pyr 95: WI 05	6024.6	1229200.0	6494.0	1470.4	268270.0
Pyr 90: WI 10	6595.1	1315200.0	5827.1	1323.6	241750.0
Pyr 80: WI 20	7645.5	1471800.0	4989.7	1137.5	207840.0
Pyr 70: WI 30	8608.8	1610600.0	4483.1	1024.1	186920.0
Pyr 60: WI 40	9512.6	1735400.0	4142.9	947.7	172770.0
Pyr 50: WI 50	10388.0	1848200.0	3898.5	892.6	162540.0
Pyr 40: WI 60	11221.0	1952400.0	3714.3	851.0	154800.0
Pyr 30: WI 70	12051.0	2049800.0	3570.5	818.5	148740.0
Pyr 20: WI 80	12879.0	2141400.0	3455.1	792.4	143870.0
Pyr 10: WI 90	13721.0	2228300.0	3360.4	770.9	139860.0
Pyr 05: WI 95	14151.0	2270300.0	3319.2	761.6	138110.0
Pyr 01: WI 99	14503.0	2303300.0	3288.7	754.7	136820.0
100% Water Ice	14592.0	2311400.0	3281.4	753.0	136510.0

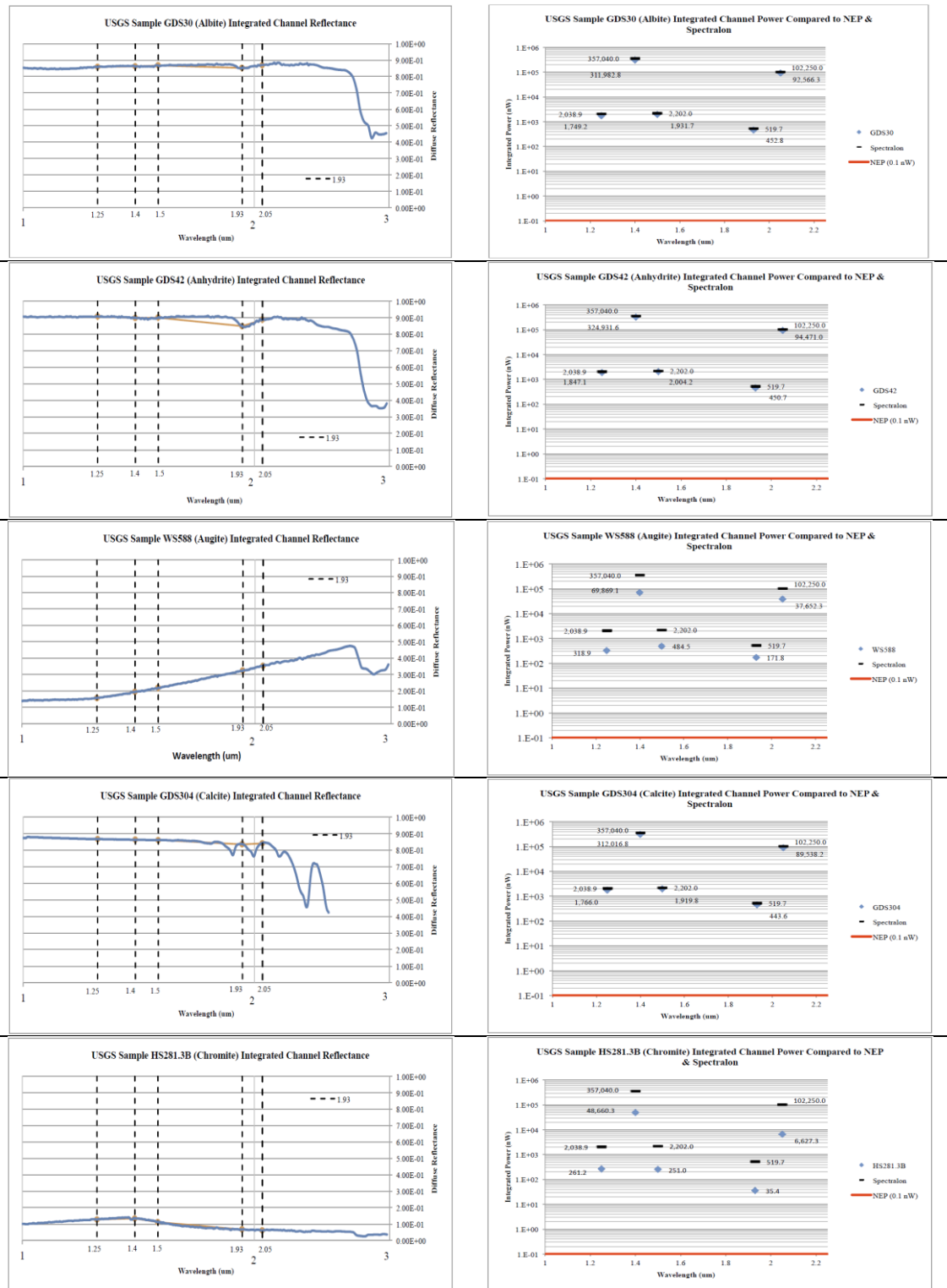
Appendix B: Additional Tables

Table B-7: Other potential analogue materials listed in Figures 2-4 and 2-5

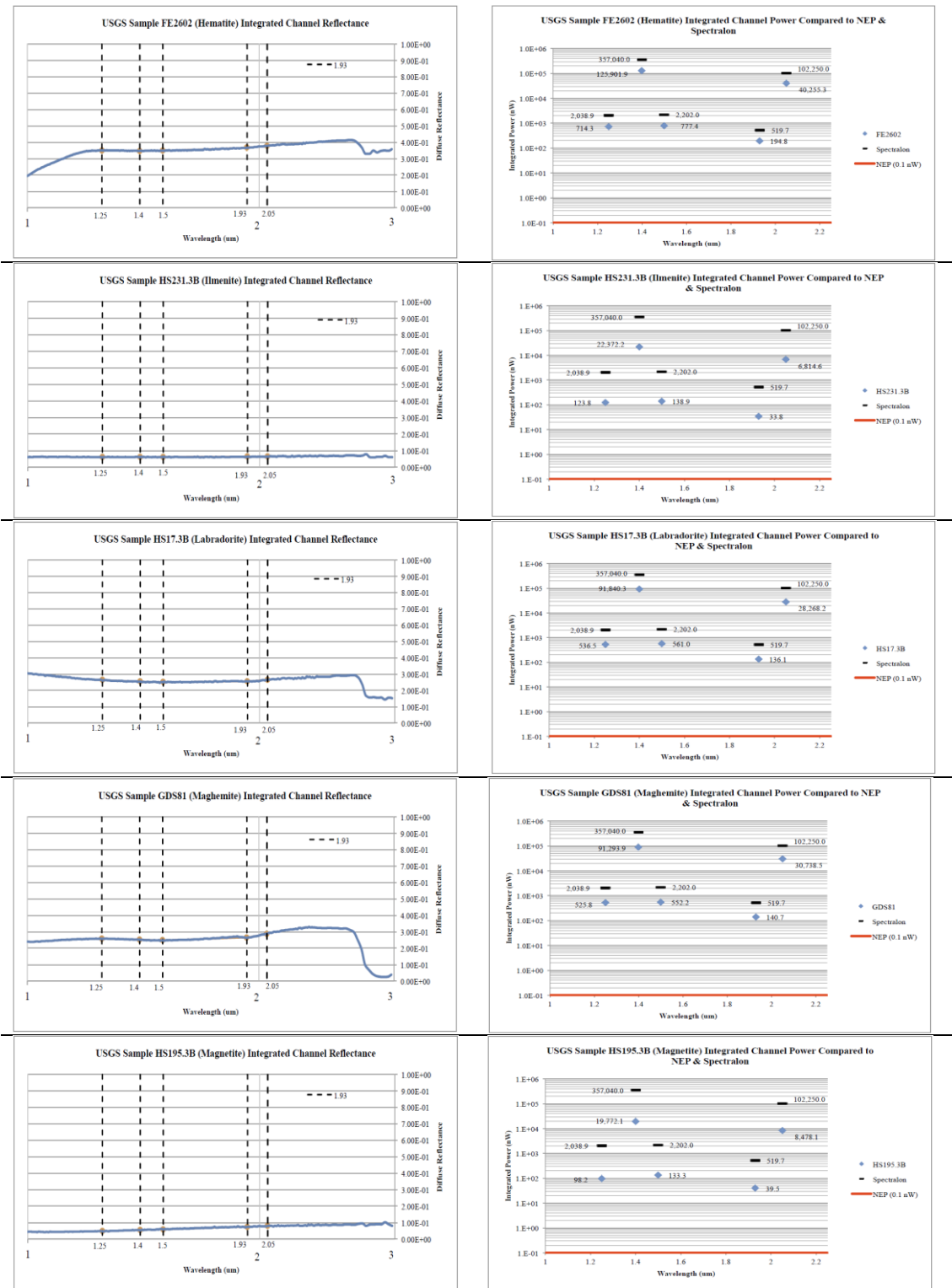
Sample	Symb.	Location: Earth	Location: Mars	Comments	References
Travertine and limestone	●	Mammoth Formation & Octopus Springs, Yellowstone National Park, WY, USA	Gusev Crater	Hydrated altered materials	Bishop et al. (2004)
Palagonite	●	Etna Volcano, Italy Skeiðara'rsandur, Iceland	General Spectral	Alternative to JSC Mars-1 from Hawaii	Esposito et al. (2000) Warner & Farmer (2010)
Montmorillonite	N/A	Wyoming	Syria & Lunae Planum	Wards	Esposito et al. (2000)
Andesite	N/A	Colorado	Various	Wards	Esposito et al. (2000)
Felsic volcanics	●	Skeiðara'rsandur, Iceland	Various	Including Andesite, dacites, and rhyolites.	Warner & Farmer (2010)
Basalt	●	Skeiðara'rsandur, Iceland Craters of the Moon Lava Field, Idaho, USA	Meridiani Planum Gusev Crater		Warner & Farmer (2010) Cornell & Hausrath (2010)
Albite	N/A	Skeiðara'rsandur, Iceland	Various		Warner & Farmer (2010)
Quartz	N/A	Skeiðara'rsandur, Iceland	Various		Warner & Farmer (2010)
Zeolites	N/A	Skeiðara'rsandur, Iceland	Various		Warner & Farmer (2010)
Beidellites	N/A	N/A	Various		Bishop et al. (2010)
Calcium carbonate			Phoenix Lander		Boyton et al. (2009)
Sulphates (altered)	●	Dixie Valley, NV, USA	Various	Ca, Si, & Al-sulphates	Housrath (Hausrath 2010)
Labradorite/halite	N/A	N/A	N/A	Reagent grade halite	Jensen & Glotch (2010)
Na-sulphate	●	Lewis Cliff Ice Tongue, Antarctica	Various		Liu and Bish (2010)
Na-borate	●	Lewis Cliff Ice Tongue, Antarctica	Various		Liu and Bish (2010)
Na-bicarbonate	●	Lewis Cliff Ice Tongue, Antarctica	Various		Liu and Bish (2010)
Ca-sulphate	●	Cerro Negro Volcano, Nicaragua	Various		Marucci et al. (2010)
Carbonates	●	Spitzbergen, Norway	Various		McAdam et al. (2010)
Jarosite	●	Olduvai Gorge, Tanzania	Various		McHenry et al. (2010)
Ferrer dolerite	●	Becon Valley, Antarctica	Various		Salvatore et al. (2010)

Note: This is just a general survey of the breadth and depth as there are a significant number of papers in the last 10 years analysing Terrestrial Analogues and comparing them to recent reported discoveries from the various Mars missions

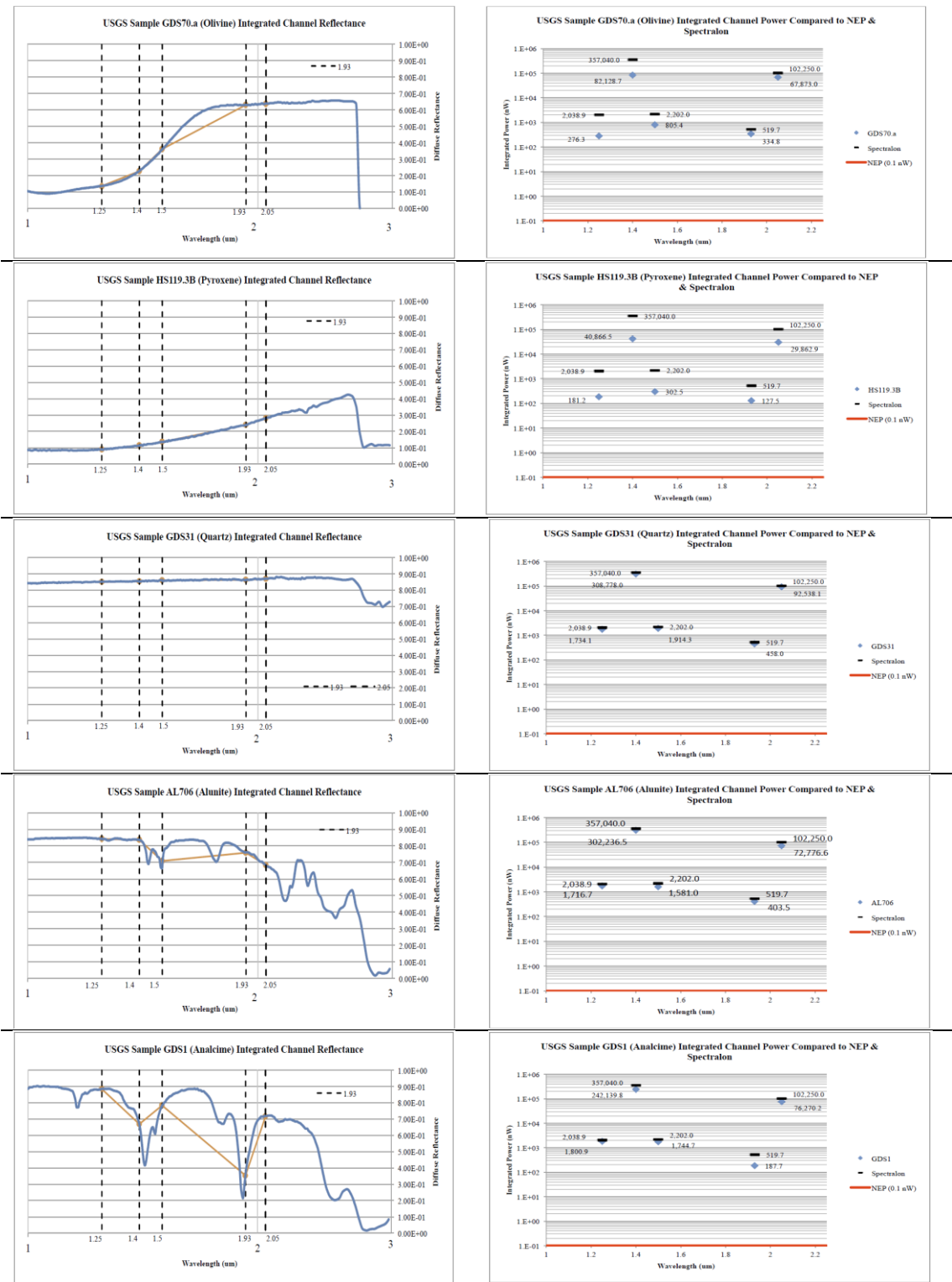
Appendix C: USGS mineral spectra and power analyses



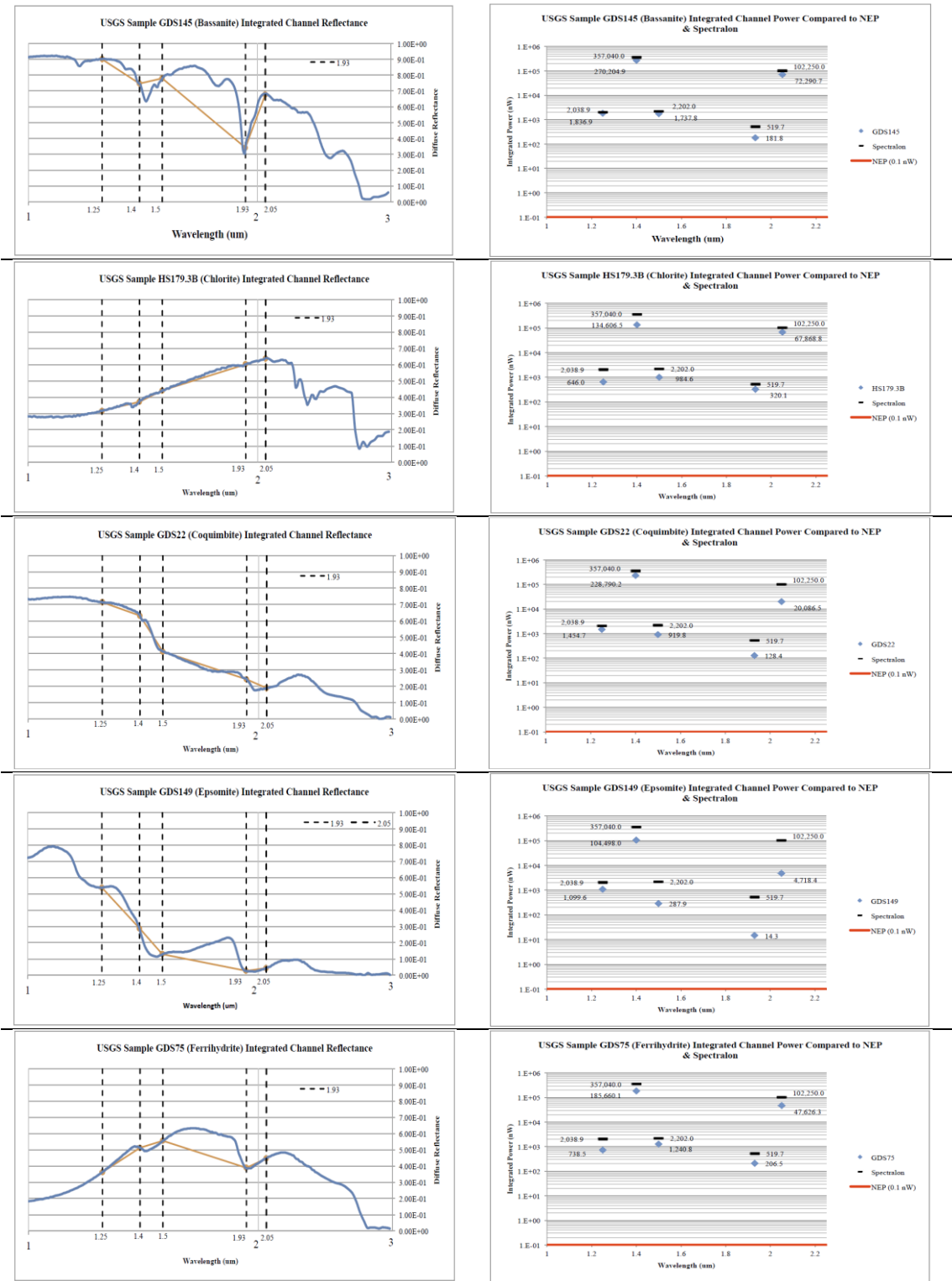
Appendix C: USGS mineral spectra and power analyses



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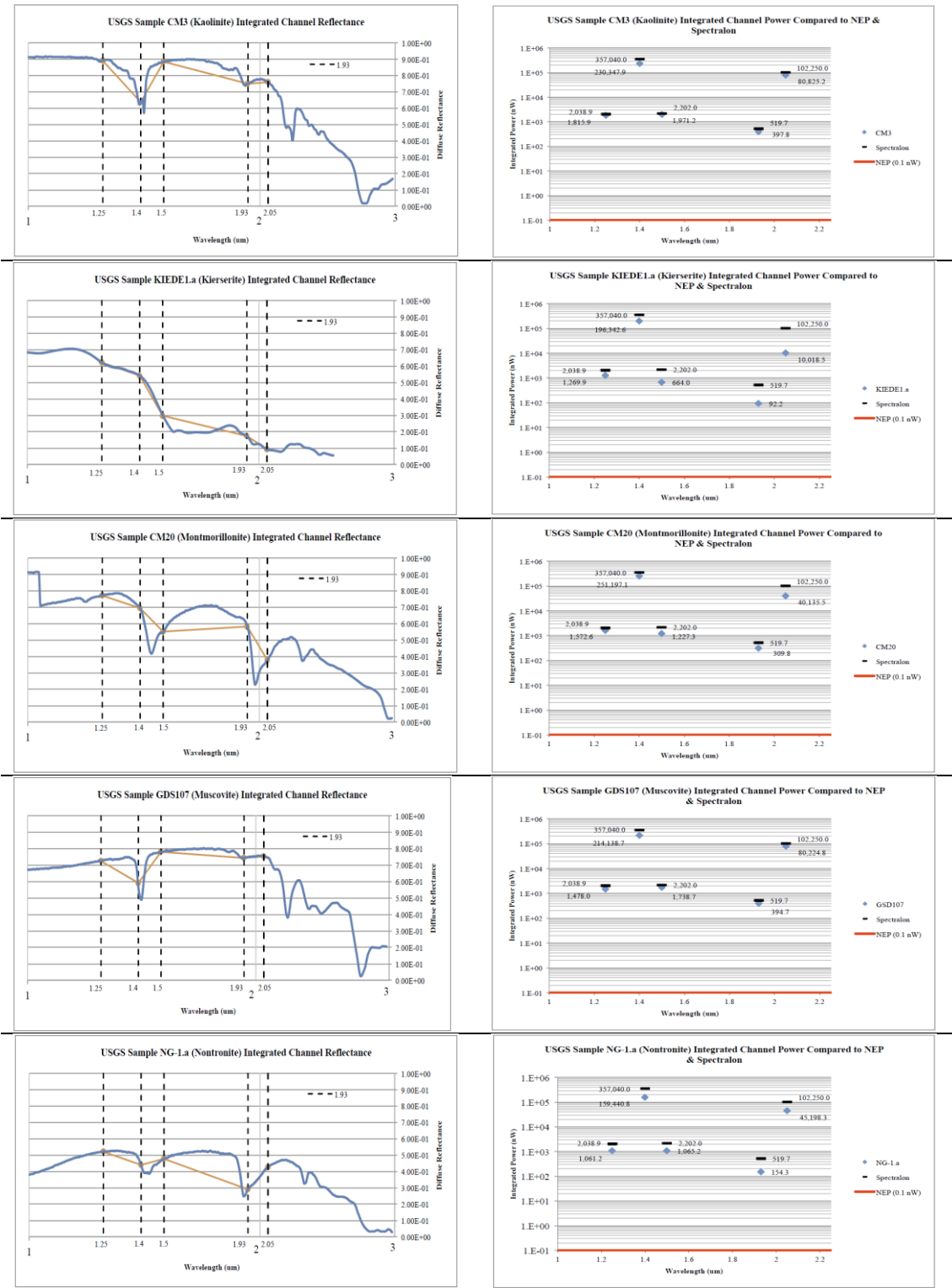
Appendix C: USGS mineral spectra and power analyses



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Appendix C: USGS mineral spectra and power analyses



Appendix D: USGS Major and Minor Minerals found on Mars downloaded 01/26/13 (un-mixed minerals)

Appendix D: USGS Major and Minor Minerals found on Mars downloaded 01/26/13 (un-mixed minerals)										Mars Specific Classes				Ref	Mars Reference							
RELAB Code	Mineral (group/variety)	Chemical Formula	Non- Hydrated	Hydrated	Bonded OH*-1	Bonded Water	Bonded H2O & OH	Phyllosilicate	Carbonate	Sulfate	Zeolite	Other Hydrated	Ferric Oxide	Other Mineral Type	Rocks of the World	Wikipedia	USGS Database	RELAB (66)	Found on Mars?	Special Note: The references have identified the indicated mineral as being present on the surface of Mars. This table does not attempt to resolve inconsistencies and disagreements from the various papers. The search is thorough, but not exhaustive. Papers might have been missed.	# Refs	
ALB	Albite	NaAlSi ₃ O ₈	1											Tectosilicate	X	X	X	1	Grassi & Formisano 2000; Maturilli 2002; Milam, 2007;	3	2	
ALM	Almandine	Fe ⁺² ₃ Al ₂ (SiO ₄) ₃	1											Nesosilicate	X	X	X	1	Morgan and Anders, 1979; Zhu et al., 2006	2	2	
ALU	Alunite	(Na,K)Al ₃ (SO ₄) ₂ (OH) ₆		1	1				1						X	X	X	1	Murchie et al., 2009; Althiede et al., 2010; Clark et al., 2008; Ehlmann et al., 2013;	4	2	
AMP	Amphibole	(Ca,Na,K)2-3(Mg,Fe2+,Fe3+,Al)5Al2Si6O22(OH)2		1	1						1			Inosilicate	X	X	X	1	Bandfield 2002; Rogers et al., 2009	2	2	
	Analcime (Zeolite)	NaAlSi ₃ O ₆ •H ₂ O		1		1				1				Tectosilicate		X		1	Ehlmann et al., 2009; Wray et al., 2009; Ehlmann, et al., 2011; Ehlmann et al, 2013;	4	2	
AND	Andesine	(Na,Ca)Al(Al,Si)Si ₂ O ₈	1											Tectosilicate	X	X	X	1	Michalski et al., 2006B; Milam, 2007;	2	2	
	Anhydrite	CaSO ₄	1						1							X		1	Clark et al., 2005; Glotch et al., 2006; Zhu et al., 2006; Squyres et al., 2004;	4	2	
ANO	Anorthite	CaAl ₂ Si ₂ O ₈	1											Tectosilicate	X	X	X	1	Popa et al., 2010; Milam, 2007;	2	2	
	Antigorite	(Mg,Fe ⁺²) ₃ Si ₂ O ₅ (OH) ₄		1	1			1								X		1	Minitti et al., 2010;	1	2	
AUG	Augite (pyroxene)	(Ca,Na)(Mg,Fe,Al,Ti)(Si,Al) ₂ O ₆	1											Inosilicate	X	X	X	1	Christensen, et al., 1998; Bandfield et al., 2000; Michalski et al., 2006B	3	2	
	Barite	BaSO ₄	1							1						X		1	Zhu et al., 2006;	1	2	
	Bassanite	2CaSO ₄ •H ₂ O		1		1				1						X		1	Wray et al., 2010; Gendrin et al., 2005; Squyres et al., 2004; Mangold et al., 2010;	4	2	
	Bloedite	Na ₂ Mg(SO ₄) ₂ •4H ₂ O		1		1				1						X		1	Squyres et al., 2004; Mangold et al., 2008;	2	2	
BRZ	Bronzite (ferroan Enstatite)	(Mg,Fe ⁺²) ₂ Si ₂ O ₆	1											Inosilicate	X	X	X	1	Christensen, et al., 1998	1	2	
	Butlerite	Fe ⁺³ (SO ₄)(OH)•2H ₂ O		1			1			1						X		1	Bishop et al., 2008;	1	2	
	Bytownite	(NaAlSi ₃ CaAl ₂)Si ₂ O ₈	1											Tectosilicate		X		1	Milam, 2007; Popa et al., 2010;	2	2	
CAL	Calcite	CaCO ₃	1						1						X	X	X	1	Christensen, et al., 1998; Ehlmann et al., 2013; Baird et al., 1976;	3	2	
	Chalcedony (Quartz)	SiO ₂	1											Tectosilicate		X		1	Mustard et al., 2008; Milliken et al., 2008;	2	2	
	Chalcopyrite	CuFeS ₂	1											Sulfide		X		1	Zhu, et al., 2006;	1	2	
CHL	Chlorite	(Mg,Fe) ₃ (Si,Al) ₄ O ₁₀ (OH) ₂ •(Mg,Fe) ₃ (OH) ₆		1	1			1							X	X	X	1	McKeown et al., 2009; Carter et al., 2009; Ehlmann et al., 2011; Ehlmann et al., 2009; Murchie et al., 2009; Clark et al., 2008; Carter and Poulet, 2012; Elhmann et al., 2013;	8	2	
CHR	Chromite	Fe ⁺² Cr ₂ O ₄	1									1			X	X	X	1	Morgan and Anders, 1979; Ming et al., 2006; McSween et al., 2008; Morris et al., 2008	4	2	
CLC	Clinocllore (Chlorite)	(Mg,Fe ⁺²) ₂ Al(Si ₃ Al)O ₁₀ (OH) ₈		1	1			1						Chlorite/Silicate	X	X	X	1	Carter et al., 2009	1	2	
	Copiapite	Fe ⁺² Fe ⁺³ ₄ (SO ₄) ₆ (OH) ₂ •20H ₂ O		1			1			1						X		1	Gendrin et al., 2005; Mangold et al., 2008;	2	2	
	Coquimbite	Fe ⁺³ (SO ₄) ₃ •9H ₂ O		1		1				1						X		1	Clark et al., 2008; Bishop et al., 2008; Mangold et al., 2008;	3	2	
	Covellite	CuS	1											Sulfide		X		1	Zhu et al., 2006;	1	2	
	Dickite	Al ₂ Si ₂ O ₅ (OH) ₄		1	1			1								X		1	Bishop et al., 2008	1	2	
DIO	Diopside	CaMgSi ₂ O ₆	1											Inosilicate	X	X	X	1	Morgan and Anders, 1979; Ming et al., 2006	2	2	
	Epidote	Ca ₂ (Al,Fe ⁺³) ₃ (SiO ₄) ₃ (OH)		1	1						1			Sorosilicate		X		1	Carter and Poulet, 2012;	1	2	
	Epsomite	MgSO ₄ •7H ₂ O		1		1				1						X		1	Gendrin et al., 2005; Squyres et al., 2004; Mangold et al., 2008;	3	2	
FHD	Ferrihydrite	5Fe ⁺³ O ₃ •9H ₂ O		1		1						1				X	X	X	1	Morgan and Anders, 1979; Carter et al., 2009; Combe et al., 2008; Farrand et al., 2009;	4	2
	Glaucinite (Mica)	(K,Na)(Fe ⁺³ ,Al,Mg) ₂ (Si,Al) ₄ O ₁₀ (OH) ₂		1	1			1								X		1	Bishop et al., 2008;	1	2	
	Goethite	alpha-FeO(OH)		1	1						1			Hydroxide		X		1	Thollot et al., 2012; Farrand et al., 2009; Ehlmann et al., 2013; Baird et al., 1976;	4	2	
GYP	Gypsum (Selenite)	CaSO ₄ •2H ₂ O		1		1				1					X	X	X	1	Gendrin, et al., 2005; Langevin et al., 2005; Murchie et al., 2009; Bibring et al., 2005; Combe et al., 2008; Altheide et al., 2010; Zhu et al., 2006; Squyres et al., 2004; Clark et al., 2008; Bishop et al., 2008; Ehlmann et al., 2013; Mangold et al., 2010;	12	2	
	Halite	NaCl	1											Halide		X		1	Squyres et al., 2004;	1	2	
HAL	Halloysite	Al ₂ Si ₂ O ₅ (OH) ₄		1	1			1							X	X	X	1	Thollot et al., 2012; Michalski et al., 2006B; Clark et al., 2008; Ehlmann et al., 2013;	4	2	
HED	Hedenbergite	CaFe ⁺² Si ₂ O ₆	1											Inosilicate	X	X	X	1	Morgan and Anders, 1979	1	2	

Appendix D: USGS Major and Minor Minerals found on Mars downloaded 01/26/13 (un-mixed minerals)

Appendix D: USGS Major and Minor Minerals found on Mars downloaded 01/26/13 (un-mixed minerals)										Mars Specific Classes				Ref				Mars Reference					
RELAB Code	Mineral (group/variety)	Chemical Formula	Non- Hydrated	hydrated	Bonded OH^-1	Bonded Water	Bonded H2O & OH	Phyllosilicate	Carbonate	Sulfate	Zeolite	Other Hydrated	Ferric Oxide	Other Mineral Type	Rocks of the World	Wikipedia	USGS Database	RELAB (66)	Found on Mars?	Special Note: The references have identified the indicated mineral as being present on the surface of Mars. This table does not attempt to resolve inconsistencies and disagreements from the various papers. The search is thorough, but not exhaustive. Papers might have been missed.	# Refs		
HEM	Hematite	alpha-Fe ₂ O ₃	1										1		X		X	X	1	Christensen, et al., 2000; Bandfield 2002; Murchie et al., 2009; Ming et al., 2006; McSween et al., 2008; McKeown et al., 2009; Combe et al., 2008; Altheide et al., 2010; Rogers et al., 2009; Zhu et al., 2006; Morris et al., 2008; Minitti et al., 2010; Squyres et al., 2004; Clark et al., 2008; Mangold et al., 2008; Ehlmann et al., 2013; Baird et al., 1976; Navrotsky et al., 2008; Bertelsen et al., 2004; Thomas and Walter, 2002;	20	2	
HEU	Heulandite	(Na,Ca) ₂₋₃ Al ₂ (Al,Si) ₂ Si ₁₃ O ₃₆ •12H ₂ O		1		1						1		Zeolite	X		X	X	1	Minitti et al., 2010;	1	2	
HBD	Hornblende (Amphibole)	Ca ₂ (Mg,Fe ⁺²) ₂ Al(Si7Al)O ₂₂ (OH,F) ₂		1	1							1		Inosilicate		X	X	X	1	Minitti et al., 2010	1	2	
APA	Hydroxyl-Apatite (Apatite)	Ca ₅ (PO ₄) ₃ (OH)		1	1							1		Phosphate	X		X		1	Ming et al., 2006; McSween et al., 2008	2	2	
HYP	Hypersthene	(Mg,Fe ⁺²)Si ₂ O ₆		1	1							1		Inosilicate	X		X	X	1	Ming et al., 2006	1	2	
ILL	Illite	(K,H ₃ O)(Al,Mg,Fe) ₂ (Si,Al) ₄ O ₁₀ [(OH) ₂ , (H ₂ O)]		1			1	1								X	X	X	1	Murchie et al., 2009; Poulet et al., 2009; Carter et al., 2009; Ehlmann et al., 2009; Minitti et al., 2010; Mustard et al., 2008B; Clark et al., 2008; Ehlmann et al., 2013;	8	2	
ILM	Ilmenite (Titanoferrite)	Fe ⁺² TiO ₃	1									1			X		X	X	1	Morgan and Anders, 1979; Ming et al., 2006; McSween et al., 2008; Morris et al., 2008	4	2	
JAD	Jadeite	Na(Al,Fe ⁺³)Si ₂ O ₆	1											Inosilicate			X	X	1	Morgan and Anders, 1979	1	2	
	Jarosite	NaFe ⁺³ ₃ (SO ₄) ₂ (OH) ₆		1	1						1						X		1	Combe et al., 2008; Farrand et al., 2009; Zhu et al., 2006; Murchie et al., 2009; Thollot et al., 2012; Squyres et al., 2004; Clark et al., 2008; Bishop et al., 2008; Ehlmann et al., 2013;	9	2	
	Kainite	MgSO ₄ •KCl•3H ₂ O		1		1						1		Halide			X		1	Lane et al., 2008; Mangold et al., 2008;	2	2	
KAO	Kaolinite	Al ₂ Si ₂ O ₅ (OH) ₄		1	1			1							X	X	X	X	1	Murchie et al., 2009; Bishop et al., 2008; McKeown, et al., 2009; Carter et al., 2009; Althiede et al., 2010; Ehlmann et al., 2009; Mustard et al., 2008B; Clark et al., 2008; Carter and Poulet, 2012; Ehlmann et al., 2013;	10	2	
	Kieserite	MgSO ₄ •H ₂ O		1		1					1						X		1	Combe et al., 2008; Zhu et al., 2006; Gendrin et al., 2005; Bibring et al., 2005; Squyres et al., 2004; Clark et al., 2008; Mangold et al., 2008; Baird et al., 1976;	8	2	
LAB	Labradorite	(NaAlSi, CaAl ₂)Si ₂ O ₈	1											Tectosilicate	X		X	X	1	Christensen et al., 1998; Michalski et al., 2006B; Milam, 2007;	3	2	
	Lizardite	Mg ₃ Si ₂ O ₅ (OH) ₄		1	1			1								X			1	Carter et al., 2009;	1	2	
	Maghemite	gamma-Fe ₂ O ₃	1									1					X		1	Hviid et al., 1997; Baird et al., 1976; Navrotsky et al., 2008; Goetz et al., 2005;	4	2	
MAG	Magnetite	Fe ⁺² Fe ⁺³ ₂ O ₄	1									1			X		X	X	1	Ming et al., 2006; McSween et al., 2008; Morris et al., 2008; Hviid et al., 1997; Baird et al., 1976; Bertelsen et al., 2004; Goetz et al., 2005;	7	2	
	Monticellite	CaMgSiO ₄	1											Nesosilicate			X		1	Zhu et al., 2006	1	2	
MON	Montmorillonite	(Na,Ca) _{0.33} (Al,Mg) ₂ Si ₄ O ₁₀ (OH) ₂ •nH ₂ O		1			1	1							X	X	X	X	1	Poulet, et al., 2005; Murchie et al., 2009; Poulet et al., 2009; Michalski et al., 2006B; Bishop et al., 2008; McKeown et al., 2009; Carter et al., 2009; Althiede et al., 2010; Clark et al., 2008; Ehlmann et al., 2013;	10	2	
MUS	Muscovite (Mica)	KAl ₂ Si ₃ O ₁₀ (OH) ₂		1	1			1							X	X	X	X	1	Murchie et al., 2009; Poulet et al., 2009; Ehlmann et al., 2009; Mustard et al., 2008B; Clark et al., 2008; Ehlmann et al., 2013;	6	2	
NON	Nontronite (Montmorillonite)	Na _{0.33} Fe ⁺³ ₂ (Si,Al) ₄ O ₁₀ •nH ₂ O		1			1	1							X	X	X	X	1	Bibring et al., 2005; Ehlmann et al., 2008; Murchie et al., 2009; Poulet et al., 2009; Bishop et al., 2008; McKeown, 2009; Carter et al., 2009; Ehlmann et al., 2009; Wray et al., 2010; Mustard et al., 2008B; Clark et al., 2008; Ehlmann et al., 2013;	12	2	
OLV	Olivine	Mg ₂ Si ₄ -Fe ₂ SiO ₄ Fo ₉₉	1											Nesosilicate	X		X	X	1	Christensen et al., 1998; Christensen et al., 2000, Bandfield 2002; Poulet et al., 2005; Murchie et al., 2009; Bibring et al., 2005; Ming et al., 2006; McSween et al., 2008; Combe et al., 2008; Skok et al., 2012; Rogers et al., 2009; Morris et al., 2008; Rogers and Aharonson, 2008; Mustard et al., 2008B; Clark et al., 2008; Bertelsen et al., 2004; Goetz et al., 2005;	17	2	
OPA	Opal	SiO ₂ •nH ₂ O		1		1						1		Tectosilicate	X		X	X	1	Murchie et al., 2009; Minitti et al., 2010; Mustard et al., 2008A; Milliken et al., 2008; Mustard et al., 2008B; Clark et al., 2008; Ehlmann et al., 2013;	7	2	
OCL	Orthoclase	KAlSi ₃ O ₈	1											Tectosilicate	X	X	X	X	1	Zhu et al., 2006	1	2	
PIG	Pigeonite	(Ca,Mg,Fe)(Mg,Fe)Si ₂ O ₆	1											Inosilicate		X	X	X	1	Skok et al., 2012	1	2	

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	Polyhalite	K ₂ Ca ₂ Mg(SO ₄) ₄ •2H ₂ O		1		1				1							X		1	Lane et al., 2008;	1	2
	Portlandite	Ca(OH) ₂		1	1							1		Hydroxide			X		1	Glotch and Rogers, Submitted;	1	2
	Prehnite	Ca ₂ Al ₂ Si ₃ O ₁₀ (OH) ₂		1	1			1									X		1	Ehlmann et al., 2011; Carter et al., 2009; Murchie et al., 2009; Ehlmann et al., 2009; Clark et al., 2008; Carter and Poulet, 2012; Ehlmann et al., 2013;	7	2
PYT	Pyrite	FeS ₂	1											Sulfide	X		X	X	1	Morris et al., 2008	1	2
PYX	Pyroxene	(Ca,Mg,Fe ²⁺ ,Fe ³⁺ ,Ti,Al) ₂ (Si,Al) ₂ O ₆	1											Inosilicate			X	X	1	Christensen et al., 1998; Bibring et al., 2005; Ming et al., 2006; McSween et al., 2008; Bandfield et al., 2000; Michalski et al., 2006B; Combe et al., 2008; Skok et al., 2012; Rogers et al., 2009; Zhu et al., 2006; Morris et al., 2008; Rogers and Aharonson, 2008; Squyres et al., 2004; Clark et al., 2008; Mangold et al., 2008; Goetz et al., 2005;	16	2
QTZ	Quartz	SiO ₂	1											Tectosilicate	X		X	X	1	Christensen et al., 1998, Rogers et al., 2009; Minitti et al., 2010;	3	2
SAP	Saponite (Montmorillonite)	(½Ca,Na) _{0.33} (Mg,Fe ⁺²) ₃ (Si,Al) ₄ O ₁₀ (OH) ₂ •4H ₂ O		1			1	1							X		X	X	1	Murchie et al., 2009; McKeown, et al., 2009; Carter et al., 2009; Minitti et al., 2010; Mustard et al., 2008B; Clark et al., 2008; Ehlmann et al., 2013;	7	2
SER	Serpentine	Mg ₃ Si ₂ O ₅ (OH) ₄		1	1			1							X		X	X	1	Carter et al., 2009; Ehlmann et al., 2011; Ehlmann et al., 2009; Ehlmann et al., 2010; Carter and Poulet, 2012; Serpentine et al., 2013;	6	2
	Stilbite	NaCa ₂ Al ₅ Si ₁₃ O ₃₆ •14H ₂ O		1		1				1							X		1	Minitti et al., 2010;	1	2
	Thenardite	Na ₂ SO ₄	1							1							X		1	Zhu et al., 2006	1	2
	Uvarovite	Ca ₃ Cr ⁺³ ₂ (SiO ₄) ₃	1											Nesosilicate			X		1	Zhu et al., 2006	1	2
	Vermiculite	(Mg,Fe ⁺² ,Al) ₃ (Al,Si) ₄ O ₁₀ (OH) ₂ •4H ₂ O		1			1	1									X		1	Carter et al., 2009;	1	2
Totals:			32	40	20	13	7	16	1	14	3	9	6						72			

Appendix E - System Error Analysis

Form of error	Description	Source of Error Data	Applicability		Estimated % Error Thermal Channel		Estimated % Error Reflectance Channel				
			Thermal	Reflectance	A	B	1.25	1.4	1.5	1.93	2.05
Spectral measurement errors											
Analog sample spectral measurement: Oxford or RELAB	Spectral properties of the sample measured with spectrometer. This error is attributed to the error associated with the spectrometer and method of this measurement.	4 wn resolution during measurement. Equates to: Channel A: 1.3%; Channel B: 0.02%; 1.25: 0.05%; 1.4: 0.06%; 1.5: 0.06%; 1.93: 0.08%; 2.05: 0.08%.	X	X	1.3	0.02	0.05	0.06	0.06	0.08	0.08
Mixing protocol	Clumping and non-linear distribution of particles in a mixed sample.	Measured data from Figure 4-10 resulted in an estimated error of about 4.4%		X	0	0	4.4	4.4	4.4	4.4	4.4
Greybody calibration target spectral characteristics	Spectral properties of the Nextel painted calibration target measured with spectrometer. This error is attributed to the error associated with the spectrometer and method of this measurement.	4 wn resolution during measurement. Equates to: Channel A: 1.3%; Channel B: 0.02%; 1.25: 0.05%; 1.4: 0.06%; 1.5: 0.06%; 1.93: 0.08%; 2.05: 0.08%.	X	X	1.3	0.02	0.05	0.06	0.06	0.08	0.08
Borehole simulator spectral characteristics	Spectral properties of the Nextel painted borehole simulator. Not measured, using Nextell calibration target spectral measurements for value. This error is attributed to the error associated with the spectrometer and method of this measurement.	4 wn resolution during measurement. Equates to: Channel A: 1.3%; Channel B: 0.02%;	X		1.3	0.02	0	0	0	0	0
Thermal Channel Emmissivity optimization error	Channel A: Reflectance calculated at .987 across the Mini-TES undisturbed bulk sample (Sol 3, P3004). Calculated error of 1.21 ± 0.12%. Channel B, Reflectance calculated as 0.929 resulting in error of 3.19±0.77%. If it is an unknown, pure mineral, errors would be max 9% and 27% for A and B, respectively. These drop to 0.02% if the sample is known	Average emissivity of samples in channel spectral response range of the 12 samples.	X		1.12	3.19	0	0	0	0	0
Spectral confusion due to shifted peaks causing false positives and negatives	Bonds causing a shift in the absorption peak that lead to a false positive or negative in mineral identification.	Natural error. Delt with in false positives and negatives assessment. No direct error attributed here.		X	0	0	0	0	0	0	0
Removal of Filters	Filters we not possible to add in this development, as tested version here.	Section 6.6 discussed the additional error associated with removal of the filters. This was estimated at 2%.		X	0	0	2	2	2	2	2
Thermal Stability											
Detector thermal stability	Fluxuations in the detector temperature leads to variations in the generated voltage and correlation to the measured surface temperature. Detector thermal variability was limited by experiment protocol. The variability was mesaured.	Measured during experiment	X		0.002	0.002	0	0	0	0	0
LED Thermal stability	fluxuations in the LED temperature lead to variations in the spectral output (peak frequency) and intensity. Not measured. Design assumes that LED will be held thermally stable and calibration will remove this artifact. The maximum variability estimated from manufacturers datasheet for a 14 deg shift was 0.045 μm, or about 2.3%	Estimated from manufacturers datasheet		X	0	0	2.3	2.3	2.3	2.3	2.3
Filter thermal stability	Everything in the FOV of the detector not at the same temperature as the detector will add/subtract energy reaching the detector from the scene. Assumed to be the same temperature as the detector with the thermal variability as measured at the detector.	Detector temperature variability measured, assumed to be the same for filter.	X		0.002	0.002	0	0	0	0	0

Appendix E - System Error Analysis

Sample/calibration target thermal stability	Variations in the scene temperature lead to variations in the generated voltage at the detector. This increases error during calibration and correlation. These were clamped to cold plate. Cold plate thermal stability dependent upon Eurotherm. Data collected according to scene temperature stability protocol. Sample/Calibration target thermal variability was measured.	Sample/Calibration target temperature was measured during the experiments. Average Stdev from testing tied to Figure 6-13 (Experiment PPTWBX9C, 01/12/13). This is 0.01 K variation and 0.005%.	X		0.005	0.005	0	0	0	0	0
Borehole simulator thermal stability	Borehole simulator clamped to surface of cold plate. Cold plate thermal stability dependent upon Eurotherm. Data collected according to scene temperature stability. Simulator variability was measured.	Borehole simulator temperatures were measured during the experiments. Average Stdev from testing tied to Figure 6-13 (Experiment PPTWBX9C, 01/12/13). This is 0.044 K variation and 0.02%.	X		0.02	0.02	0	0	0	0	0
Component Errors											
Filter spectral response range	Filters were measured with spectrometer, so spectrometer measurement error	Spectrometer/method estimate		X			0.05	0.06	0.06	0.08	0.08
Detector window spectral response range	Window was not possible to measure. Estimated error.	Estimated error.	X	X	0.5	0.5	0.5	0.5	0.5	0.5	0.5
Electrical noise	Line noise from assembly and component manufacturing variability.	Estimated error.	X	X	1	1	1	1	1	1	1
LED spectral response range	Due to manufacturers variability	Estimated error.		X	0	0	1	1	1	1	1
Detector variability	Due to manufacturers variability	Manufacturers datasheet	X		0.05	0.05	0.05	0.05	0.05	0.05	0.05
Design Errors											
Detector positioning	Instrument manufacturing tolerances causing detector to not be orthogonal to surface. Calibration should factor this out to zero, since this is a static, non-moving component.	Estimated	X	X	0	0	0	0	0	0	0
LED positioning	Instrument manufacturing tolerances causing LED to not be in correct position to surface, changing the peak reflection reaching detector. Calibration should factor this out to zero, since this is a static, non-moving component.	Estimated	X	X	0	0	0	0	0	0	0
Instrument positioning in bore-hole	Instrument is smaller than borehole, so it could be placed such that the detector is not orthogonal to the surface. This would change the reflectance angle. Since the calibration is dependent upon positioning, if the position is different between measurement and calibration, this will cause an error. Shouldn't be an error for the thermal channels as it uses the detector full FOV.	Estimated		X	0	0	0	0	0	0	0
System Error											
Measured System Error	The measured system error reported in Table 6-4 and Section 6.9.	Measured during thermal and reflectance experiments	X	X	0.08	0.08	2.5	2.5	2.5	2.5	2.5
Root-mean-square:							6.10	6.10	6.10	6.10	6.10
Thermal Channel RMS Error for Mini-TES sample P3004:							2.75	3.38			
Thermal Channel RMS Error if measuring pure, known sample:							2.52	1.12			
Thermal Channel RMS Error if measuring pure, unknown sample:							9.35	27.02			