A NOVEL THERMAL INFRARED SPECTRAL MODEL FOR TESTING THE UNCERTAINTIES IN REMOTE MINERAL ABUNDANCE RETRIEVALS: IMPLICATIONS FOR REMOTE SENSING INVESTIGATIONS. C. S. Edwards¹, C. Pilorget², M. M. Osterloo³; ¹Northern Arizona University, Department of Physics and Astronomy, NAU BOX 6010, Flagstaff, AZ 86011, USA, Christopher.Edwards@nau.edu; ²Institut d’Astrophysique Spatiale, CNRS/Université Paris-Sud, 91405 Orsay, France; ³Laboratory for Atmospheric and Space Physics, University of Colorado Boulder, Boulder, Colorado, USA.

Introduction: Remote compositional investigations in the middle infrared wavelength (e.g. 6-50 µm) region have long relied upon the assumption of linear mixing of end-members to determine surface mineralogy. Variations of this technique have been successfully applied to both Earth and Mars laboratory and remotely acquired data. However, the majority of studies have targeted samples that were composed of grain sizes larger than ~60 µm. Initial work of Ramsey and Christensen [1] demonstrated that mixing remains linear to ~60 microns, using 250-500 µm size fractions as endmembers. That study concluded that below this threshold, the linear retrieval algorithm fails. However, the authors present evidence that suggest when appropriate endmember spectra for corresponding mixtures are provided for the algorithm, linearity continues to 10-20 µm size fractions. This conclusion was based on a relatively simple binary mixture of quartz and andesine rather than more representative mineral mixtures or multi-component mixtures.

Additional work by [2] carried out manual point counts of the minerals present in 96 thin sections of rock samples to determine their abundances, measured the thermal infrared emission spectrum of the same section and then used the linear unmixing algorithm of Ramsey and Christensen [1] with a library of spectral endmembers appropriate for the sample to verify the uncertainties in mineral abundance retrievals. Additional updates to the numerical model of Ramsey and Christensen [1] was carried out by Rogers and Aharonson [3], where the authors provided a non-negative least squares fitting routine that simultaneously solved the set of linear equations without relying on an iterative approach used previously [1]. This work, while foundational, has several potential issues which must be addressed to achieve a more robust understanding of the uncertainties and limitations of this method. Of note is that the samples of Feely and Christensen [2] were all solid rock samples, with cut surfaces, eliminating the effects of surface roughness, thin alteration coatings, and particulates that have the potential to significantly affect the retrieved abundances. Additionally, potential temperature gradients in surfaces composed of fine particulates [4, 5], change the strength and position of the Christiansen Feature [e.g. 6].

Furthermore, it is not practical to test the limits of linear mixing purely in the laboratory as multi-component mixtures as geologically complicated surfaces cannot be readily constructed. Similarly, simulating complex spectral mixtures has proved to be a challenge due to the complex nature of models and the requirements of optical constants. To date, there has been no comprehensive study to investigate the limitations of linear deconvolution or offer an alternative approach for determining surface compositions of remote bodies.

In this work, we present a novel forward spectral model that allows the creation and spectral simulation of mixtures without 1) the use of the optical constants for each endmember (n; refractive index and k; extinction coefficient) or 2) the spectral emissivity measured for each endmember. This model will permit the formation of many more simulated mixtures that can be tested against traditional retrievals such as the commonly used linear unmixing algorithms.

Methods:

Laboratory Measurements: To develop inputs for our forward spectral model, we acquired data of two spectral mixtures. This limited endmember dataset (Figure 1) acquired at Arizona State University’s Thermal Emission Spectroscopy Laboratory using a Nicolet

![Figure 1](top) mixtures of quartz (left), hematite (right) and a 50/50 wt% mixture (center) of the two endmembers. (bottom) TIR spectra of the quartz and hematite mixtures. Increase.
Nexus 670 spectrometer following the methods of [7] using minerals from the [8] spectral library. In this pilot study, mixtures of two different phases (quartz and hematite, due to their primarily non-overlapping spectral features; and forsterite and albite, due to their significantly overlapping spectral features) were created by 10 wt% intervals from 0-100% with grain sizes from 710-1000 µm to avoid the effects described by Ramsey and Christensen [1]. These samples were then heated to 80°C and measured in the emission spectrometer above. Spectra of the quartz and hematite mixtures are presented in Figure 1. As the first quality control measure, the two endmembers (quartz and hematite) were used as endmembers in the spectral unmixing library for the 50/50 wt% mixture and using the method of [3] resulted in abundance of 52.25±1.4% Hematite and 47.75±0.1% Quartz.

Model Description: The TIR spectral model that has been developed is directly inherited from [9]. The latter is a Monte-Carlo model capable of simulating the radiative transfer in the VIS-NIR from the grain scale to the sample/surface scale in a 3D environment. The same methodology was applied here, except that the photons in the TIR model are directly emitted by the different grains (instead of originating from an external source in the VIS-NIR model). The photons are then scattered until they reach the surface or are absorbed. Geometric optics is assumed, meaning that the grain size is at least several times greater than the wavelength. The medium is defined by a given grain size distribution and by optical properties that can be unique for each grain. The grains are then set in a grid, allowing for the creation of spatial heterogeneities at specific locations within the medium (e.g., understanding a specific grain in mixtures including linear, intimate, and/or layered). The radiative transfer is then calculated using a ray tracing approach between the grains including probabilistic scattering parameters such as single scattering albedo and a phase function at the grain level. This allows for significantly faster computation times than classical ray tracing models.

The model was tested using optical constants as inputs, but also spectral emissivity data. In particular, it is possible to link the bulk emissivity with the grain emissivity that should be use to recreate the endmember spectrum. Fig. 3 illustrates the capability of the model to simulate a 50-50% intimate mixture of hematite and quartz using the spectral emissivity data obtained for each endmember.

Discussion and Next Steps: We have developed a novel model that is capable of simulating various geologically relevant surfaces, including mixtures such as linear, intimate or layered. Further testing will provide robustness and applicability of the model for future quantitative mineralogical analyses of remotely acquire TIR spectra. In the next steps of this work we will: 1) continue validating this model as a tool for generating spectral mixtures, 2) simulate multiple mixtures (binary, ternary etc.) using a range of endmembers with both distinct and overlapping spectral features, and 3) unmix the model data in order to assess the sensitivity of these mixtures while also considering instrument noise common to infrared spectrometers.