EXACT CALCULATION OF THE SCATTERING PROPERTIES OF WAVELENGTH-SIZED PARTICULATES J. A. Arnold[1], T. D. Glotch[1] and M. J. Wolff[2], [1]Stony Brook University (255 Earth and Space Sciences, Stony Brook University, Stony Brook, NY 11794-2100), [2] Space Science Institute (Space Science Institute, Milwaukee, WI)

Background: Mid-IR emissivity spectra of regolith-type surfaces are highly dependent on particle size. At present, scattering models are not fully able to replicate this dependence, limiting our interpretations of mineralogical composition and abundance.

Moersch and Christensen (1995) [1] evaluated four different radiative transfer (RT) models in comparison to measured emission spectra of fine-grained quartz. Of these, the Mie/Hapke hybrid model [2] comes closest to reproducing changes in IR spectra with particle size. However, these changes are still underestimated for the strongest bands. Mustard and Hays (1997) [3] concentrated on using Mie/Hapke reflectance to model olivine and quartz grains <25μm in size, representing the finest fraction of the lunar and martian regoliths. This was largely successful in the case of olivine. The results for quartz, however, were mixed, with the largest discrepancies occurring between 7.3μm and 9.5μm, just long-ward of the Christiansen frequency (an emissivity maximum that occurs in the mid-IR when the index of refraction of a substance approaches that of the surrounding medium). Mustard and Hays concluded that the model may break down due to the large values of n and k quartz exhibits in this region.

The Mie/Hapke hybrid model uses the scattering properties of an isolated sphere to determine two of the inputs needed in a RT model: the single scattering albedo (w) and the asymmetry parameter (g). For this approach to be valid, any interaction between the emitted waves of individual particles within a cluster must be assumed to take place in the far-field. This criterion is satisfied in low-density media, such an atmosphere, but not within a planetary regolith. Pitman et al. (2005) [4] introduced a more thorough treatment of particle packing by using a discrete-ordinate-method instead of a 2-stream approximation. They also included a better characterization of grain size distribution. Despite these improvements, there are still significant discrepancies between model and laboratory spectra. The two main reasons cited for these shortcomings were 1) the need for a more realistic treatment of particle shape and 2) models better able to deal with closely-packed particles as would be found in a typical regolith.

Scattering properties of particle clusters: In this work, we address the latter problem by incorporating the T matrix approach to look at the average scattering properties of clusters containing large numbers of particles. This method, based on the direct computation of solutions to Maxwell's equations, is able to deal with multiple scattering [5] of closely packed particulates. The T matrix relates the incident radiation to the scattered radiation and depends solely on the intrinsic properties of the scattering material (shape, size, refractive index) and orientation with respect to the coordinate system, rather than the incident or reflected field. This allows for rapid calculation of scattering properties over a many different illumination angles [6].

Mishchenko et al. 2007 [7], used this method to examine the scattering properties of sphere clusters of increasing density. A spherical volume element of fixed radius was filled with randomly-distributed wavelength-sized particles. The number of particles within the volume element was varied to give packing densities of 0.1%-24%. At low density, the results of the T-matrix method are in agreement with standard RT models, while the onset of multiple-scattering effects becomes apparent at higher density.
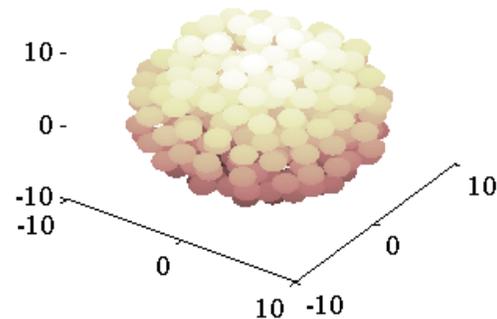

Fig 1: Plot produced from the MSTM input file containing the sphere coordinates.

Methods and Computing Resources: The Multiple Sphere T Matrix (MSTM) package developed by D. Mackowski, which is available at [http://eng.auburn.edu/users/dmckwski/scatcodes/], calculates the scattering properties of clusters containing spherical particles [8], in a similar manner to Mischenko (2007) [7], described above. To run this code we are utilizing the New York Blue/P supercomputer at Brookhaven National Laborotory along with the Seawulf Cluster housed on the Stony Brook campus. NY Blue/P has up to 512 nodes

available for a given job, while the Seawulf Cluster has 30 nodes available for an individual user. Both machines have 2GB of memory per node.

Using the MSTM package, we calculated the scattering properties of quartz spheres over a range of wavelengths and particle sizes. To do this, we set up a volume element of 300 spheres with 30% packing efficiency (Fig 1). The size parameter ($kR=2\pi R/\lambda$) is adjusted to correspond with the wavelength and particle radius and the quartz optical constants are taken from Wenrich and Christensen (1996) [9].

Results: The code outputs scattering and total extinction efficiencies (Q_{scatt} and Q_{ext}) for the whole cluster of particles. From these, we can calculate the single scattering albedo ($\mathcal{W}$) as $\mathcal{W}=Q_{scatt}/Q_{ext}$.. We then derive hemispherical emissivity from $\mathcal{W}$ according to Hapke 1993b [2]:

$$\varepsilon = \frac{2\gamma}{1+\gamma}\left(1+\frac{1}{6}\frac{1-\gamma}{1+\gamma}\right) \quad \text{where} \quad \gamma = \sqrt{1-w}$$

Once converted to emissivity, the results of the MSTM calculations can be compared to laboratory emissivity spectra of quartz powders whose grain size ranges are known (Fig 2).
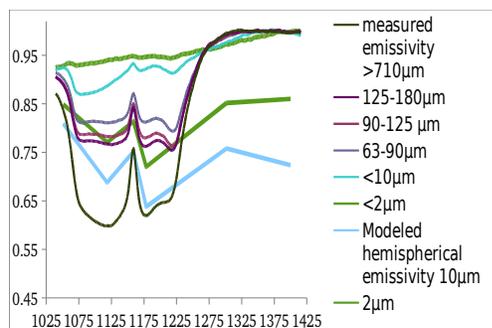

Fig 2: 6-point emissivity spectra of clusters of 10μm and 2μm diameter quartz spheres generated from MSTM calculations plotted with laboratory spectra of powdered quartz.

We can also look at how the scattering phase function varies with the complex index of refraction. Fig 3 shows the difference between small and large values of k.

Discussion and future work: While the calculated emissivity spectra show clear changes with particle size, they do not duplicate the drastic decrease in spectral contrast seen in laboratory spectra for very fine particulates (<10μm). There are several possible avenues for improvement. We will repeat these calculations with clusters of more realistic packing density. Building on this, we would also like simulate a particle size distribution within the volume element. With only 300 particles, the size parameter of the volume element rapidly becomes small compared to the wavelength of incident radiation. To extend this method to longer wavelengths we will have to increase both the size of the volume element and the number of

spheres. This generally increases the computation time, although at longer wavelengths/smaller size parameters computational time can be substantially reduced. Hence, the most feasible solution to this issue may be to adjust the target cluster for each wavelength. Lastly, it would be beneficial see how Hapke models compare with other RT formulations when using MSTM calculations as input.

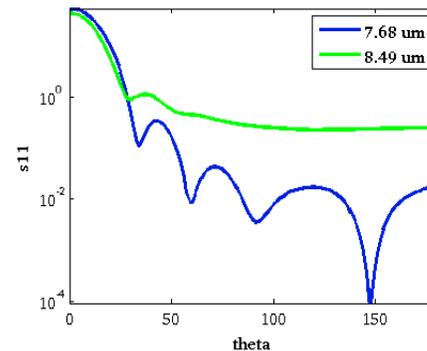**Fig 3: Normalized scattering phase function of a cluster of 2μm diameter quartz spheres for two different wavelengths of the incident beam. At 7.68μm n=0.846 and k=0.050, while at 8.49μm n=0.109 and k=1.090**

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