LIMITATIONS OF EFFECTIVE MEDIUM APPROXIMATIONS FOR SPECTRAL MODELING OF SPACE WEATHERED PARTICLES. C. Legett IV[1], T. D. Glotch[1], and P. G. Lucey[2], [1]Stony Brook University, 255 Earth and Space Sciences Building, Stony Brook, NY 11794-2100 carey.legett@stonybrook.edu, [2]Hawaii Institute of Geophysics and Planetology, University of Hawaii, 2525 Correa Rd., Honolulu, Hawaii 96822.

Introduction: Calculating the light scattering properties of heterogeneous and/or irregular particles is a computationally difficult process that is, in some cases, beyond the capability of current computing resources to complete in a reasonable amount of time. Due to this complexity, it is common to use simplifying assumptions to reduce the computational requirements. One of the most common of these simplifying techniques is the use of effective medium approximations (EMAs). EMAs operate on the assumption that a heterogeneous particle can be represented as a homogeneous particle with "effective" optical properties that are calculated from the properties of the original components. Mishchenko et al. (2016) [1] found the use of EMAs to be appropriate for certain compositions and geometries of heterogeneous aerosol particles where the size parameter ($x = 2\pi r/\lambda$) of the inclusions in a host particle was very small and where there were only small differences in the complex refractive indices between the inclusions and host particle. They found that by the time the size parameter of the inclusions reached x=0.5 (in host particles with x=4 and x=8), significant errors were present in their models due to the use of the EMA. Given that these size parameters are similar to those of geometrically complex space weathered particles in the lunar regolith, we attempt to determine the applicability of the commonly used [e.g. 2, 3] Maxwell-Garnett EMA (MGEMA) [4] to models of the light scattering properties of the lunar regolith fines. Of particular importance to this work is the fact that MGEMA takes only the optical constants of the two phases and the volume fraction of the inclusions into account. It does not account for the particle size of the inclusions.

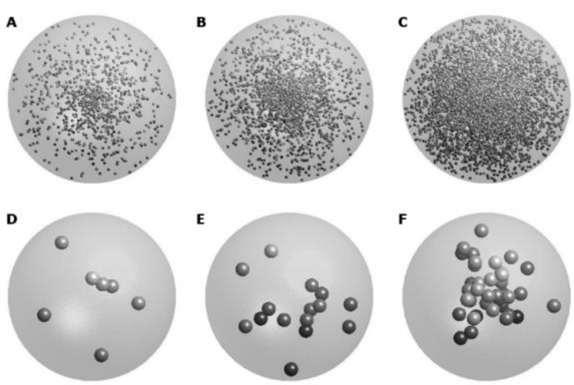

Figure 1. 3D renders of the six model cases: A) 20 nm Fe, 1 wt%, B)20 nm Fe, 2 wt%, C) 20 nm Fe 5 wt%, D) 100 nm Fe 1 wt%, E) 100 nm Fe 2 wt%, F) 100 nm Fe 5 wt%.

Methods: We generated six model cases, each representing a 1200 nm diameter olivine host sphere containing 1, 2, or 5 wt% metallic iron as randomly placed 20 or 100 nm diameter inclusions (Figure 1). We then used the MGEMA to generate effective optical constants at 10 nm steps between wavelengths of 500 and 2500 nm. Olivine optical constants were computed by us from a San Carlos olivine powder using the Shkuratov geometric optics model [5]. Iron optical constants were provided by [6]. These single sphere cases were then run through a Mie code [7] that we ported to Python. This model provided the scattering and extinction efficiencies (Q_{sca} and Q_{ext} respectively), and the S_1 and S_2 elements of the 2x2 amplitude scattering matrix for a scattering angle of 150° from which we calculated the S_{11} element of the 4x4 scattering matrix by:

$$S_{11} = \frac{1}{2}(|S_1|^2 + |S_2|^2)$$

The S_{11} parameter provides information about the angular distribution of scattered energy. An angle of 150° was chosen to mimic a typical spacecraft viewing geometry with an incidence angle 30° off the vertical, and a vertical emergence angle.

We then used the Multiple Sphere T-Matrix Model (MSTM) [8] to calculate the scattering properties of the original particles before simplification via MGEMA. MSTM provides an exact, numeric means of solving the time-harmonic Maxwell equations for clusters of spherical particles. This allowed us to calculate the scattering properties of the geometrically complex particles without relying on the simplifications necessary for the Mie method. MSTM provided Q_{ext}, Q_{sca}, and S_{11} for each original particle.

Finally, we ran the single-sphere MGEMA particles through MSTM to show that both the simple Mie model and MSTM provided identical outputs given the same inputs.

From the scattering parameters provided by the Mie and MSTM models, we calculated a reflectance value using Hapke's IMSA [9] equation:

$$r(i,e,g) = \frac{\varpi}{4\pi}\frac{\mu_0}{\mu_0 + \mu}[p(g) + H(\mu_0)H(\mu) - 1]$$

where μ_0 and μ are the cosines of the incidence and emergence angles. ϖ is the single scattering albedo (SSA):

$$\varpi = \frac{Q_{sca}}{Q_{ext}}$$

and H is an approximation of the Amartsumian-Chandrasekhar H function,

$$H(x) = \frac{1+2x}{1+2x\sqrt{1-\varpi}}$$

The p(g) term is the *phase function* and corresponds to the S_{11} parameter output by MSTM. We determined that due to differences in notation, the S_{11} parameter calculated from the Mie model differs from that output by MSTM as:

$$p(g) = S_{11,MSTM} = \frac{4\pi S_{11,Mie}}{C_{sca}k^2}$$

where C_{sca} is the scattering cross section, and k is the wavenumber.

Results and Discussion: In all six cases, the MGEMA runs resulted in broadly overestimated SSA and reflectance values compared to MSTM. This effect was worst in the 900-1300 nm range but was significant above ~700 nm. The MGEMA/Mie models matched the MGEMA/MSTM output exactly for all runs. The best-case overestimation of reflectance was for the 20 nm inclusions at 1 wt%, which still exceeded 10% above the MSTM value at short wavelengths (Figure 2). The worst-case overestimation of reflectance was for the 100 nm inclusions at 5 wt% at nearly 70% above MSTM calculated values near 1100 nm with everything above ~800 nm having greater than a 20% higher reflectance (Figure 3). Due to this overestimation in the MGEMA/Mie cases, the reflectance spectra were redder for the MGEMA/Mie than the MSTM runs. This effect was more pronounced for the 100 nm diameter inclusions than for the 20 nm diameter inclusions.

The shape of the reflectance spectra for these cases were primarily controlled by the "wiggles" and "ripples" in the scattering and extinction efficiencies that are inherent in a single sphere case [10]. Even though the MSTM model runs contained up to several thousand inclusions, and are therefore not strictly single sphere runs, the scattering properties of the 1200 nm diameter host dominate. The fact that these model spectra do not resemble typical remote sensing data or bulk laboratory data is expected. These models represented the simplest possible cases with which to examine the differences in the scattering properties calculated by the two methods.

Conclusions: The fact that the diameter of the iron particles had a significant effect on the resulting reflectance spectra means that the key assumption of the MGEMA does not hold for these particles: that only the optical constants and volume fraction of the phases present are important. We demonstrated that this assumption, that the particles are all small enough with respect to the wavelength (size parameters of 0.025 for 20 nm particles and 0.13 for 100 nm particles under 2500 nm illumination) that their exact size can be neglected introduced significant errors in both the overall albedo as well as the slope of the modeled spectra. Using the MGEMA/Mie combination to model space weathered particles may result in those models underestimating the reflectance and overestimating the slope of the visible and near infrared reflectance, depending on the nature of multiple-particle scattering interactions beyond the scope of these cases.

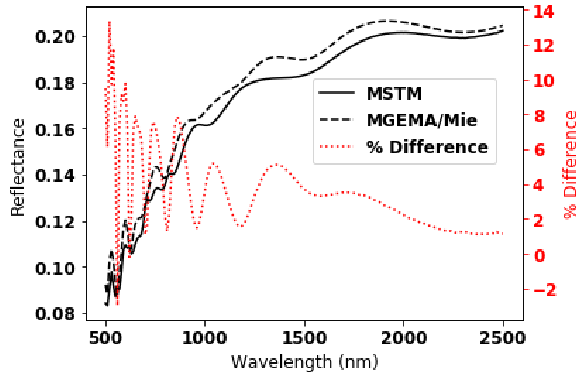

Figure 2. Reflectance comparison between MSTM and Mie/MGEMA models for the 20 nm diameter inclusions at 1 wt% Fe. The % difference is relative to the MSTM run.

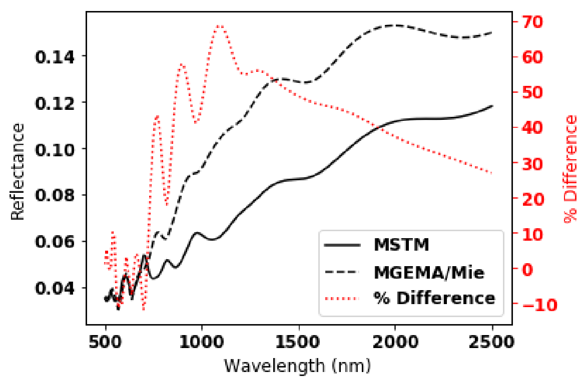

Figure 3. Reflectance comparison between MSTM and Mie/MGEMA models for the 100 nm diameter inclusions at 5 wt% Fe. The % difference is relative to the MSTM run.

References:

[1] Mishchenko et al. (2016) *JQSRT*, *178*, 284-294. [2] Hapke B. (2001) *JGR-Planet*, *106*, 10039-10073. [3] Lucey P. & Riner M. (2011) *Icarus*, *212*, 451-462. [4] Bohren C. & Huffman D. (1983) *Absorption and Scattering of Light by Small Particles* [5] Shkuratov Y (1999) *Icarus*, *137*, 235-246 [6] Cahill et al. (2018) *Icarus*, *317*, 229-241 [7] Mätzler C. (2002) *MATLAB Functions for Mie Scattering and Absorption* [8] Mackowski D. & Mishchenko M (2011) *JQSRT*, *112*, 2182-2192 [9] Hapke B. (2012) *Theory of Reflectance and Emittance Spectroscopy* [10] van de Hulst H. (1957) *Light Scattering by Small Particles*