A MONTE CARLO APPROACH TO RADIATIVE TRANSFER SPECTRAL UNMIXING. K. M. Cannon[1] and J. F. Mustard[1], [1]Brown University, Department of Earth, Environmental, and Planetary Sciences, Providence RI, 02912. Email: kevin_cannon@brown.edu

Introduction: Radiative transfer models (RTMs), including the Hapke [1] and Shkuratov [2] methods, have been used to quantitatively unmix both laboratory and remote spectra, simultaneously determining mineral abundances and particle sizes [e.g., 3-5]. Parameters in the Shkuratov model include the optical constants n and k, the effective optical pathlength S (here defined as $\langle D \rangle = xD$ where D is the particle diameter and x depends on particle shape), and the filling factor q; the Hapke model also includes viewing geometry and the internal scattering coefficient s. Some of these parameters can be constrained on a sample-by-sample basis through careful laboratory measurements [6], or are estimated and kept internally consistent to determine optical constants of samples and then then unmix physical mixture suites of those same samples [7]. However, it is rarely possible to measure all these parameters for remotely sensed data. Here, we embrace this uncertainty in the model parameters by employing a Monte Carlo approach to spectral unmixing.

Methods: We solve for abundance and particle size using the Hapke model [1], assuming n and k can be determined for mineral endmembers. Free parameters include s and x, as well as the type of phase function used (Legendre polynomial vs. single lobe Henyey-Greenstein function) and the phase function coefficients. These free parameters are independently and randomly chosen from normal distributions with bounding values derived from the literature (e.g., Figures 9 and 10 in [8]). Each set of free parameter values gives a different unmixing result, and therefore a different point on a plot of particle size vs. abundance for each endmember (see Fig. 2). By performing thousands of unmixing iterations, a cloud of points is built up that reflects solution regions for each endmember instead of a single point that would come from estimating each of the model parameters. This Monte Carlo approach is somewhat analogous to the so-called MCU model used in terrestrial remote sensing [9], although in that case it is the endmembers themselves that are randomized instead of the model parameters.

We first applied this Monte Carlo technique to two different three-component physical laboratory mixtures from the RELAB database: anorthite, enstatite and olivine (hereafter Series 1) [8], and magnesite, nontronite and olivine (Series 2) [10]. Optical constants were derived for the endmember components using the Hapke model, assuming n is constant with wavelength (Fig. 1). The k values for the Series 1 endmembers all fall in quite similar ranges, while the Series 2 endmembers have a wider spread in values (Fig. 1b). We then ran 5000 unmixings of a spectrum from a single physical mixture of the endmember minerals: 42% anorthite, 42% enstatite and 16% olivine (by mass) for Series 1, and 16% magnesite, 68% nontronite and 16% olivine for Series 2.

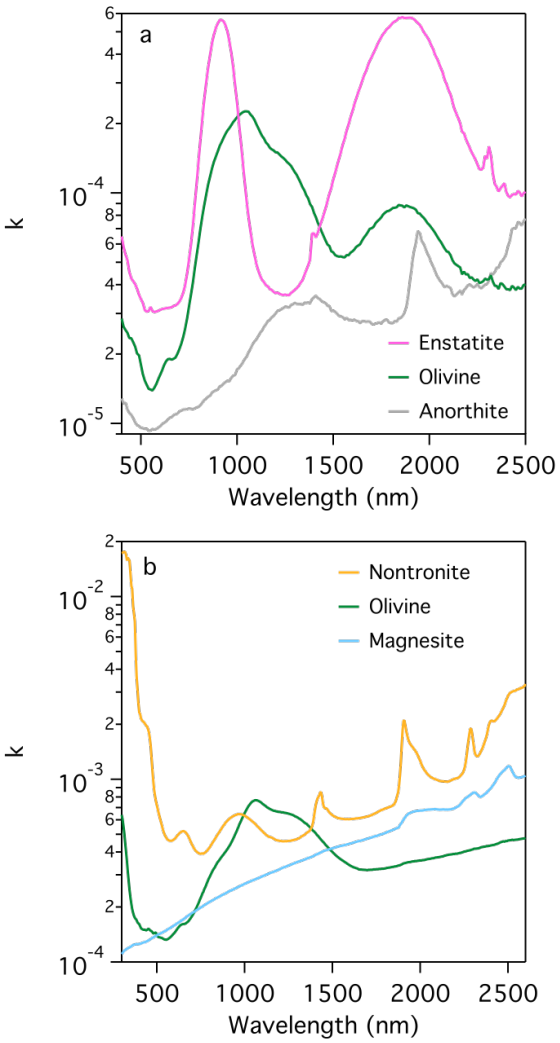

Figure 1. Derived k spectra for Series 1 (a) and Series 2 (b) endmembers.

Results: Figure 2 shows Monte Carlo unmixing results for the mixtures, plotted in particle size versus volume abundance. Figure 2a shows that Series 1 is relatively well-behaved, with most results falling in a single cluster with a limited spread in modeled abun-

dance. There is a much larger spread in particle size, with points extending upwards of >10^6 μm. Importantly, the actual measured amounts of each endmember in the mixture lie close to the largest Monte Carlo point clusters, and close to the two points obtained from using common choices for the Hapke parameters (*s*=0; Legendre polynomial phase function with *b*=-0.4, *c*=0.25; *x*=0.2 for irregular particles, ~0.9 for spherical particles [7]).

The situation differs markedly for Series 2. Figure 2b shows that instead of a single cluster for each endmember, there are 3-4 clusters that together cover abundance ranges of ~30%. In this case, there are no points from the Monte Carlo unmixing that approach the actual measured values in both abundance and particle size, although there are unmixing results that simultaneously give abundances within 5% of the actual values for all endmembers (but at highly unrealistic particle sizes).

Discussion: The preliminary results here suggest that caution should be taken when using RTMs to quantitatively unmix remote spectra. In Series 2 the RTM was unable to obtain accurate abundances and particle sizes simultaneously, even though this was a carefully controlled laboratory experiment with only three endmembers. On the other hand, the RTM works quite well for Series 1, perhaps giving false confidence that it can be applied to remote datasets using >3 endmembers.

In Series 2 the non-uniqueness of the solutions presented itself as multiple clusters within the plot of particle size versus abundance, in contrast to Series 1 (Fig. 2). These types of clusters might be useful to determine a range of possible solutions for remote unmixing, even though in the example of Series 2 none of the clusters coincided with the actual measured values. Future work will apply this technique to more mixture suites, attempt to determine why the model behaves so differently in Series 1 and Series 2, and eventually apply the technique to remote datasets.

References: [1] Hapke B. (1981) *JGR*, *86*, 3039. [2] Shkuratov Y. et al. (1999) *Icarus*, *137*, 235. [3] Poulet F. et al. (2009) *Icarus*, *201*, 69. [4] Li S. and Milliken R. E. (2015) *MAPS*, *50*, 1821. [5] Liu Y. et al. (2016) *JGR*, *121*, 2004. [6] Sklute E. C. et al. (2015) *Am. Min.*, *100*, 1110. [7] Robertson K. et al. (2016) *Icarus*, *277*, 171. [8] Mustard J. F. and Pieters C. M. (1989) *JGR*, *94*, 13619. [9] Asner G. P. and Lobell D. B. (2000) *Remote Sens. Env.*, *74*, 99. [10] Ehlmann B. L. et al. (2011) *EPSC-DPS Joint Meeting*, vol.6.

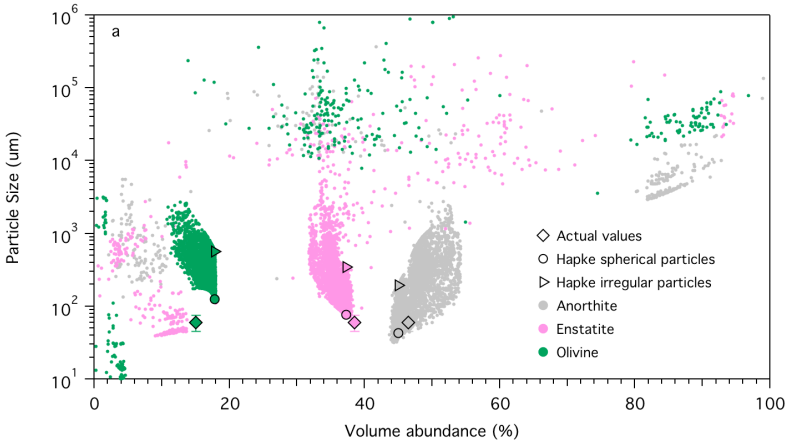

Figure 2a. Plot of particle size versus abundance for the Monte Carlo unmixing of the Series 1 mixture spectrum. Each point represents one of the unmixing results for a different set of randomly chosen model parameters.

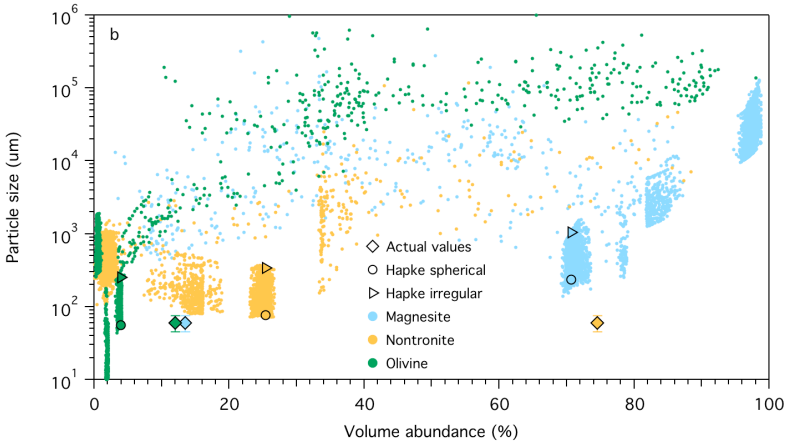

Figure 2b. Same as 2a but for Series 2. Notice the multiple solution clusters and greater degree of scatter in the results.