

A NEW OPEN-SOURCE HAPKE RADIATIVE TRANSFER PROGRAM FOR DETERMINING OPTICAL CONSTANTS AND ANALYZING PHASE BEHAVIOR. E. C. Sklute¹, D. Domingue-Loren¹, T. D. Glotch², M. Rucks³, and C. Ye², ¹Planetary Science Institute, 1700 E. Fort Lowell Rd Ste 106, Tucson, AZ 85719, ecsklute@psi.edu, ²Stony Brook University, Dept. of Geosciences, 255 ESS Building, Stonybrook, NY. ³Princeton University, Dept. of Geosciences. Guyot Hall, Princeton, NJ 08544.

Introduction: The interaction of light with a particulate medium produces a spectrum that is dependent upon multiple variables, such as composition, grain size, surface roughness, scattering angle, and packing density, to name a few. Extracting this wealth of information requires that the individual contributions to that spectrum can be deconvolved. One of the most theoretically robust and popular methods for spectral deconvolution in systems and at wavelengths where linear mixing does not occur, is the application of radiative transfer (RT) theory, specifically the treatment outlined by Bruce Hapke [1, 2].

Hapke's treatment of RT theory explicitly models contributions of singly and multiply scattered light from properties like composition, grain size, phase angle, internal scattering, and packing density. The model is iteratively minimized against the data to determine the most reasonable (mathematically) values for these variables, thus providing *quantitative* information about the target material. Most often, the quantitative parameter of interest is the composition. For this application, the optical constants, *i.e.*, the real and imaginary indices of refraction (n and k), for all potential phases in a mixture must be known. To date, use of the model has been limited by the lack of appropriate optical constants for many materials [3].

Because RT theory can be used to model spectra from optical constants, it can also be used to derive optical constants from spectra of pure mineral end members. Using RT theory in this way, however, requires that constraints exist to separate phase and grain size contributions from the material's intrinsic scattering and absorption properties (optical constants). Multiple grain size and phase angle spectra are often used to this end [4], however, the solutions are still often non-unique.

Here, we present a modification to the methods presented in Sklute et al., 2015 [4], inspired by the methodology of Yang et al., 2019 [5], that better isolates these individual spectral contributions. This new open-source code thus delivers more robust solution and can facilitate the expansion of the available library of optical constants. As an added benefit, the first sections of the new, multi-part procedure can be used analyze the phase behavior of any system for which multiple phase angle spectra exist.

Theory: For a particulate material with porosity, P ,

incidence angle, i , emergence angle, e , and phase angle, g , the reflectance of a sample with filling factor

$K = -\ln(1 - 1.209(1 - P)^{(2/3)})/1.209(1 - P)^{(2/3)}$, ratioed to the reflectance of a Lambertian scatterer viewed under the same geometry is [2]:

$$REFF(i, e, g) = K \frac{w}{4} \frac{1}{\mu_0 + \mu} \left\{ [1 + B(g)]p(g) + H\left(\frac{\mu_0}{K}\right)H\left(\frac{\mu}{K}\right) - 1 \right\}.$$

Here, μ and μ_0 are the cosines of i and e , respectively, $H(x)$ is an approximation of the Ambartsumian-Chandrasekhar H-function [2,6]:

$H(x) \approx \left\{ 1 - wx \left[r_0 + \frac{1-2r_0x}{2} \ln\left(\frac{1-x}{x}\right) \right] \right\}^{-1}$, or its exact solution. The variable $r_0 = (1 - \gamma)/(1 + \gamma)$ is the diffuse reflectance and $\gamma = \sqrt{1 - w}$ is the albedo factor. The single scattering albedo for a densely packed medium is

$$w \cong Q_s = S_e + (1 - S_e) \frac{(1 - S_i)}{1 - S_i \theta},$$

where S_i and S_e are Fresnel reflectances for internally and externally scattered light, respectively and can be approximated by:

$$S_i \approx 1.014 - \frac{4}{n(n+1)^2}; S_e \approx \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} + 0.05.$$

The variable, θ , is the internal transmission factor:

$$\theta = \frac{r_i + \exp(-\sqrt{\alpha(\alpha+s)}(D))}{1 + r_i \exp(-\sqrt{\alpha(\alpha+s)}(D))}, \text{ where } r_i = \frac{1 - \sqrt{\alpha/(\alpha+s)}}{1 + \sqrt{\alpha/(\alpha+s)}},$$

(D) is the apparent grain size, s is the internal scattering factor, and $\alpha = 4\pi k/\lambda$ is the absorption coefficient. The phase dependence of singly scattered light can be modeled in multiple ways, including one- or two-term Legendre Polynomials, and single or double Henyey-Greenstein functions. Finally, the imaginary part of the index of refraction, k , can be related to the real part of the index of refraction, n , via a singly subtractive Kramers-Kronig (SSKK) transformation:

$$n(\lambda) = n(\lambda_0) + \frac{2(\lambda^2 - \lambda_0^2)}{\pi} \times P \int_0^\infty \frac{\lambda' k(\lambda')}{[\lambda^2 - (\lambda')^2][\lambda_0^2 - (\lambda')^2]} d\lambda'.$$

Methods: It can be seen from the equations above, that the phase dependence of the singly scattered light is isolated to the first parenthetical term of **REFF**, whereas grain-size dependence is isolated in the single scattering albedo, w . Thus, multiple phase angle spectra of the same grain size can be assumed to have the same single scattering albedo, and minimization of this set of spectra assumes nothing about the grain size or the optical constants. It simply requires that all spectra of the same grain size have the same single scattering

albedo and that all spectral variation be accounted for by the phase function and the backscatter function (if it is used, typically only for phase angles $<15^\circ$). Once this step is performed, the wavelength- and grain-size-dependent phase functions can be assumed constant for the rest of the computation. This section also quickly and easily determines phase behavior from multiple phase-angle spectra of the same material or scene (Figures 1-3).

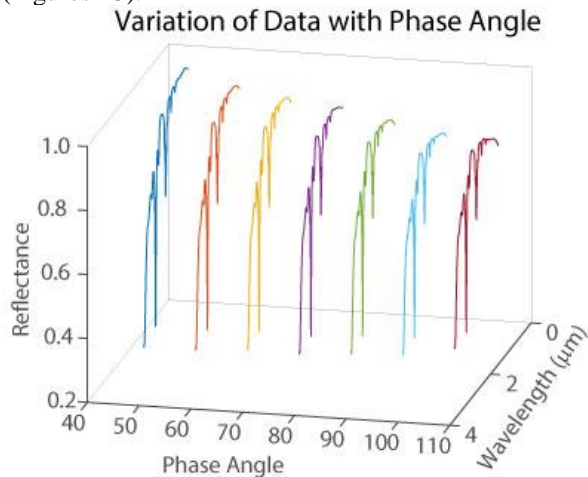


Figure 1. Spectral variation with wavelength and phase angle for bassanite (125-180 μm). Program plot from Section 6.

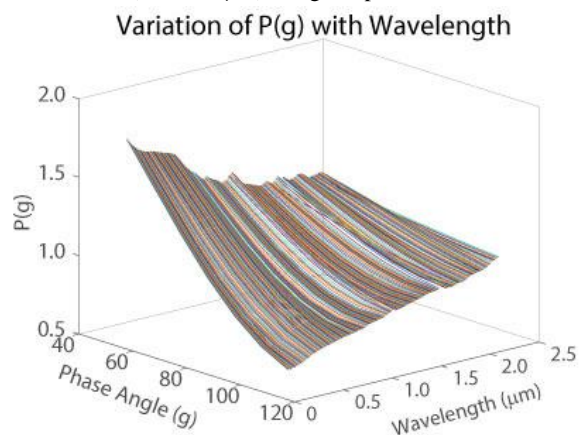


Figure 2. Variation of $P(g)$ with wavelength and phase angle for bassanite (125-180 μm) modeled with a 2-term Legendre Polynomial. Program plot from Section 6.

Next, multiple grain size spectra all taken at the same phase angle are used to compute k by assuming n is a constant (average value at the sodium D line) and requiring that all spectral variations between the grain sizes are accounted for by optimizing apparent grain size, $\langle D \rangle$, and internal scattering coefficient, s , for each spectrum.

This wavelength-dependent, k , is then combined with MIR k data (although an option exists to use it on its own) to perform an SSKK transformation to derive the wavelength-dependent n . This new n is then used to

minimize again for k , and these steps are repeated several times until variation between subsequent iterations is minimal (Figure 4).

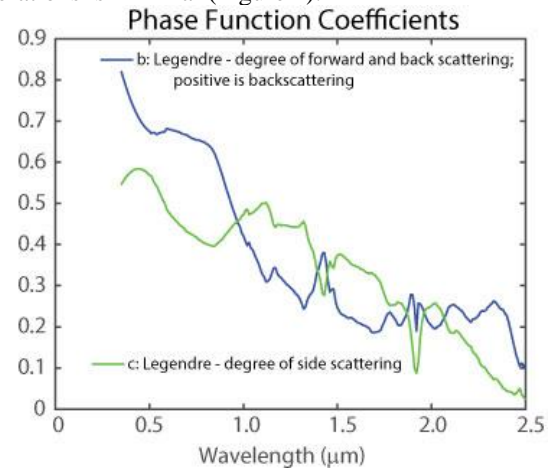


Figure 3. Phase function coefficients of two-term Legendre Polynomial plotted in Figure 2. Program plot from Section 6.

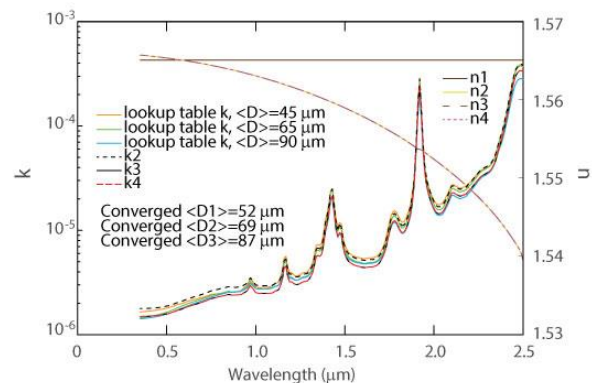


Figure 4. Derived n and k values for iterations 1 thru 4 of the minimization of bassanite $i=45$, $e=-20$, $D1=90-125 \mu\text{m}$, $D2=125-180 \mu\text{m}$, $D3=180-250 \mu\text{m}$. Lookup table values for k s calculated from individual spectra using scalar values of b , c , and n are shown for comparison.

Conclusions: We have created a new version of the Sklute et al. MatLab code for the derivation of optical constants from multi-grain size, multi-phase angle spectra. The open-source code is available at zenodo.org doi:10.5281/zenodo.4429127. The latest version can be obtained ecsklute@mtholyoke.edu

References: [1] Hapke, B. (1981) *JGR*, 86, 3039–3054. [2] Hapke, B. (2012) Cambridge University Press, UK, 507p. [3] Clark, R. N. (2018) *Europa Deep Dive 2*, Abstract #3027. [4] Sklute E. C., et al. (2015) *Am. Mineral.*, 100, 1110-1122. [5] Yang, Y. et al. (2019) *JGR-Planet.*, 124, 31-60. [6] Chandrasekhar, S. (1960) Dover, New York.

Acknowledgements: This work was supported, in part, by the NASA RISE2 SSERVI team and NASA PDART seed funding, award #80NSSC18K0528.