

**WEB-BASED, OPEN SOURCE, VISIBLE AND NEAR INFRARED OPTICAL CONSTANT DETERMINATION OF GEOLOGIC MATERIALS.** E. C. Sklute<sup>1</sup>, C. Carey<sup>2</sup>, M. D. Dyar<sup>1</sup>, and T. G. Glotch<sup>3</sup>,<sup>1</sup> Mount Holyoke College, 50 College St. South Hadley, MA. 01075, ecksklute@mtholyoke.edu, <sup>2</sup>College of Information and Computer Sciences, University of Massachusetts, 140 Governor’s Drive, Amherst MA 01003, <sup>3</sup>Stony Brook University, 255 ESS Building, Stony Brook, NY. 01094-2100.

**Introduction:** Quantitative determination of the mineral phases on planetary surfaces is critically important to constrain models of planetary surface mineralogy and geology. However, in the visible and near-infrared (VNIR 0.35-2.5 μm) wavelength region, increased multiple scattering events lead to a nonlinear relationship between spectral response and composition, such that linear spectral unmixing is not possible. Yet many of the relevant remote sensing instruments used to analyze planetary surfaces (Casini VIMS, MEX OMEGA, MRO CRISM, and AVIRIS) cover the VNIR wavelength range. Therefore, quantitative interpretation of these data sets requires explicit models of the interactions of light with particulate matter. For intimately mixed surfaces where grain size is much greater than the wavelength of light used for the observation (the geometric optics regime), radiative transfer (RT) theory can be applied to extract quantitative mineral abundances if the optical constants (the real and imaginary indices of refraction, *n* and *k*) for all minerals in the mixture are known. To facilitate the determination of optical constants for a broad range of minerals relevant to planetary sciences, the open source MatLab computer code described in [1] is being converted to an open source, web-based code written in Python, therefore requiring no paid software to run.

**Theory:** For a particulate material with porosity, *P*,  $K = -\ln(1 - 1.209(1 - P)^{(2/3)})/1.209(1 - P)^{(2/3)}$  and radiance is

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

The bracketed term takes into account contributions from single scattering events (left), assumed isotropic multiple scattering events (middle), and losses from absorption (right). Here, *H*(*x*) is an approximation of Ambartsumian-Chandrasekhar’s H-function [2]:

$$H(x) = \left\{ 1 - [1 - \gamma]x \left[ r_0 + \left( 1 + \frac{1}{2}r_0 - r_0x \right) \ln\left(\frac{1-x}{x}\right) \right] \right\}^{-1},$$

*r*<sub>0</sub> = (1 - *γ*)/(1 + *γ*) is the diffuse reflectance, and *γ* = √(1 - *w*) is the albedo factor [3]. The single scattering albedo is

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

where *S<sub>i</sub>* and *S<sub>e</sub>* are Fresnel reflectances for internally and externally scattered light, respectively. These 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,

such that,  $\theta = \frac{r_i + \exp(-\sqrt{\alpha(\alpha+s)\langle D \rangle})}{1 + r_i \exp(-\sqrt{\alpha(\alpha+s)\langle D \rangle})}$ , where

$$r_i = \frac{1 - \sqrt{\alpha/(\alpha+s)}}{1 + \sqrt{\alpha/(\alpha+s)}}, \alpha = 4\pi k/\lambda$$

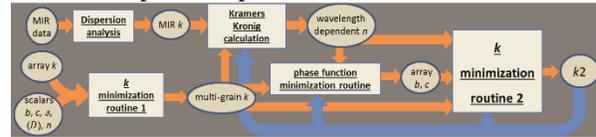
is the absorption coefficient, *⟨D⟩* is the apparent grain size, and *s* is the internal scattering factor. The phase dependence of singly scattered light can be modeled with a Legendre polynomial [4], such that:

$$p(g) = 1 + b \cos(g) + c(1.5 \cos^2(g) - 0.5).$$

The imaginary part of the index of refraction, *k*, can be related to the real part of the index of refraction, *n*, via a Kramers-Kronig transformation:

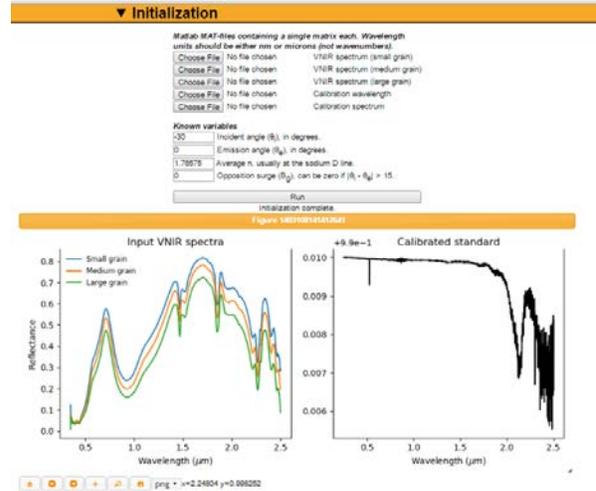
$$n(\lambda) = n(\lambda_0) + \frac{2(\lambda^2 - \lambda_0^2)}{\pi} \times P \int_0^\infty \frac{\lambda' k(\lambda')}{[\lambda^2 - (\lambda')^2][\lambda_0^2 - (\lambda')^2]} d\lambda'.$$

**Program:** The graphical interface walks through the same steps as the previous MatLab version.

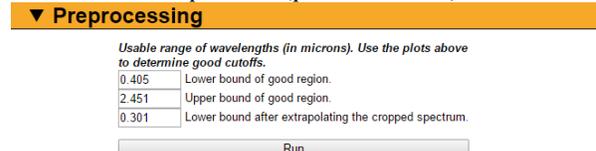


Data for potassium jarosite are shown:

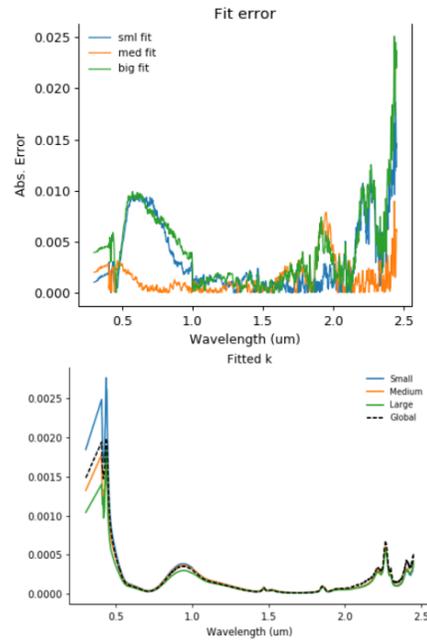
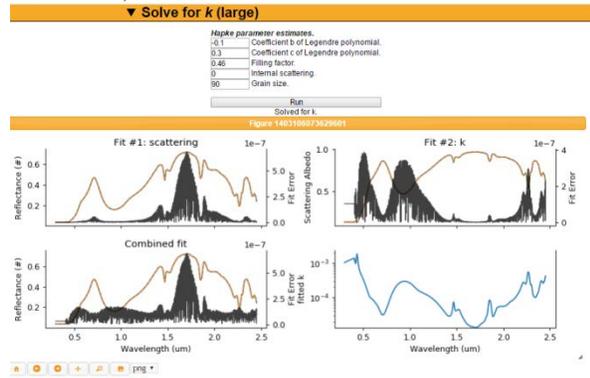
1. Data Selection.



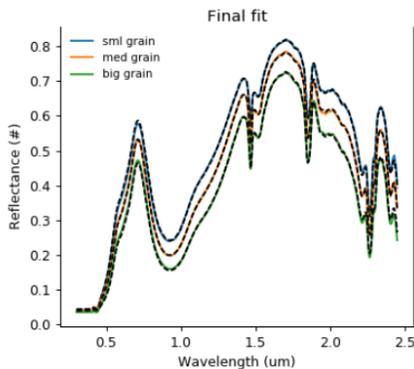
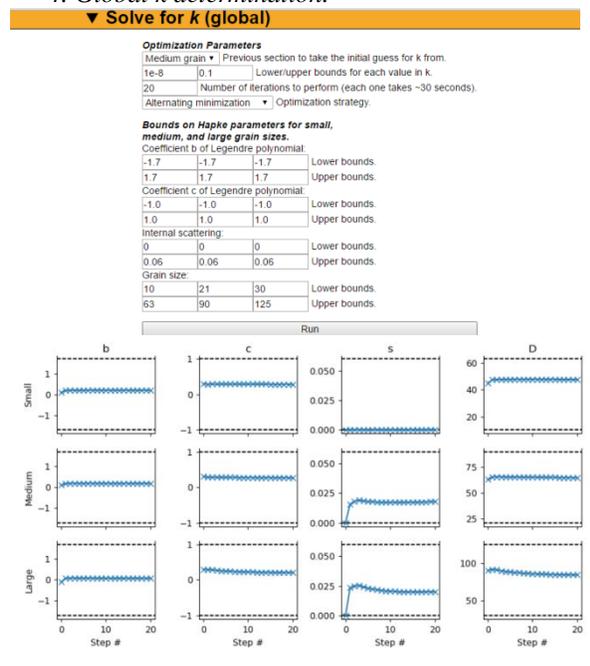
2. Data Manipulation (plot not shown).



3. Look-up table  $k$  determination (only one grain size shown).



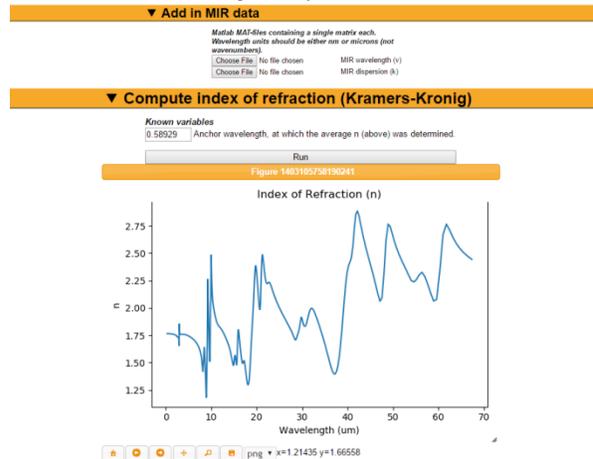
4. Global  $k$  determination.



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**References:** [1] Sklut, E. C., et al. (2015) *Am. Mineral.*, 100, 1110-1122. [2] Chandrasekhar, S. (1960) Dover, New York. [3] Hapke, B. (2002) *Icarus*, 157, 523-534. [4] Mustard, J. F. and Pieters, C. M. (1989) *JGR*, 94, 13619-13634.

4. Kramers Kronig transformation.



Each graph is interactive and downloadable. Although the code is not interactive in the same way as the MatLab version, it is still fully modifiable and completely free to use. The final web interface will be available at: <http://nemo.cs.umass.edu:44322/>.

**Future work:** The program is currently being updated to include the latter steps of phase function determination, with a choice of phase functions. After the phase function section is successfully integrated, the program will be modified to allow iterative minimizations between the  $k$ ,  $n$ , and phase function sections. The next year of troubleshooting and testing should make this interface a streamlined and accessible method for optical constant determination.