

**OPCON.MTHOLYOKE.EDU: A WEB-BASED TOOL FOR DETERMINATION OF VNIR OPTICAL CONSTANTS FROM MULTI-GRAIN-SIZE, MULTI-PHASE-ANGLE POWDERED MINERAL SPECTRA.** A. Sudhakar<sup>1</sup>, E. C. Sklute<sup>2</sup>, C. Carey<sup>1</sup>, T. D. Glotch<sup>3</sup>, and M. D. Dyar<sup>2,4</sup>, <sup>1</sup>Univ. of Massachusetts, College Inform. & Computer Sci., 140 Governors Dr., Amherst, MA 01003, [aish.sspls@gmail.com](mailto:aish.sspls@gmail.com), <sup>2</sup>Planetary Science Inst., 1700 E. Fort Lowell Rd., Tucson, AZ 85719, [ecsklute@psi.edu](mailto:ecsklute@psi.edu), <sup>3</sup>Stony Brook Univ., 255 ESS Building, Stony Brook, NY 01094, <sup>4</sup>Mount Holyoke College, Dept. of Astronomy, 50 College St., South Hadley, MA 01075.

**Introduction:** Extending the suite of web-based tools that facilitate high-level scientific research is an important facet of improving the accessibility, efficiency, and transparency of projects funded by the government and non-profits. While intellectual products of federally funded work are public domain, the accessibility and functionality of these products to the scientific community and general public can always be increased. Creating web-based tools to allow a user to explore and model scientific data can engage a wider audience than tools for which specialized software is required.

As examples, Google Mars and associated tools, like Arizona State University's Mars Image Viewer (<http://viewer.mars.asu.edu>), have made the wealth of Martian data accessible to experts and non-experts alike in an interactive and easy to use format. Our group has spent the past decade building the DEVAS (Data Exploration, Visualization, and Analysis for Spectroscopy; <http://nemo.mtholyoke.edu>) website. Its interactive, python-encoded platform consolidates many of the larger spectral databases and enables users to upload their own spectra and browse, match, pre-process, and baseline-correct thousands of spectra across a variety of spectroscopic techniques [1]. The website, Mösstool (<http://mosstool.com/>), which covers the specialized field of Mössbauer spectroscopy, allows users to interactively fit either server hosted or user supplied spectra, as well as learn about the technique.

Here we present the latest version of a python-encoded, web-based tool (<http://opcon.mtholyoke.edu>) for derivation of visible and near infrared (VNIR) optical constants from variable grain-size and multiple phase-angle spectra. This product is based upon the open-source Matlab code created by E. Sklute [2], and leverages the ongoing collaboration between Sklute, Stony Brook Geosciences (Glotch Lab), Mount Holyoke College Astronomy (Dyar Lab), and The University of Massachusetts, Amherst, College of Information and Computer Science. It is produced in an effort to support an increase in the number and availability of optical constants and encourage more theoretical development.

**Theory:** Quantitative determination of mineral and glass phase proportions on planetary surfaces is needed to place critical constraints on models of planetary surface composition. In the VNIR, increased multiple scattering events mean spectral response is not a linear

function of composition, i.e., linear spectral unmixing is not possible. Because many remote sensing instruments used to analyze planetary surfaces (e.g., Casini VIMS, MRO CRISM, Chandrayaan-1 M<sup>3</sup>, OSIRIS-REx OVIRS, and AVIRIS) cover the VNIR wavelength range, quantitative interpretation of these data sets requires explicitly modelling the interaction of light with particulate matter. For intimate mixtures with grain sizes much greater than the wavelength, radiative transfer (RT) theory can be used to determine quantitative mineral abundances if the optical constants (the real and imaginary indices of refraction,  $n$  and  $k$ ) for all materials in the mixture are known. The popular Hapke formulation of RT theory [3] states that for a particulate material with porosity,  $P$ ,

$$K = -\ln(1 - 1.209(1 - P)^{(2/3)})/1.209(1 - P)^{(2/3)}$$

and reflectance of a medium viewed illuminated at angle  $i$ , and viewed at angle  $e$  ratioed to the reflectance of a Lambertian scattered illuminated and viewed at the same angles is:

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

Here,  $\mu$  and  $\mu_0$  are the cosines of  $i$  and  $e$ , respectively,  $H(x)$  is an approximation of Ambartsumian-Chandrasekhar's H-function [3,4]:

$H(x) \approx \left\{ 1 - wx \left[ r_0 + \frac{1-2r_0x}{2} \ln\left(\frac{1-x}{x}\right) \right] \right\}^{-1}$ , 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 are 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,  $\theta$ , is the internal transmission factor:

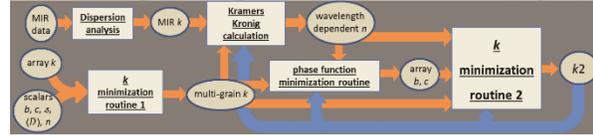
$$\theta = \frac{r_i + \exp(-\sqrt{\alpha(\alpha + \delta)\langle D \rangle})}{1 + r_i \exp(-\sqrt{\alpha(\alpha + \delta)\langle D \rangle})}, \text{ where } r_i = \frac{1 - \sqrt{\alpha/(\alpha + \delta)}}{1 + \sqrt{\alpha/(\alpha + \delta)}}$$

$\langle D \rangle$  is the apparent grain size,  $\delta$  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 sub-

tractive Kramers-Kronig (SSKK) transformation:

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

**Program:** The graphical interface walks through the same steps as the previous MatLab version (Fig. 1).



**Figure 1.** Flow diagram of grammatical elements.

**Data Selection.** Available modeling choices allow the user to use or ignore  $B(g)$ , to assume that spectralon is Lambertian or isotropic, and to perform the computation using either an approximation for the  $H$ -function, or exact values from lookup tables. The user interface allows for the inclusion of up to ten grain size spectra.

**Pre-processing.** Pre-processing plots the data and allows the user to cut off noise and model the data farther into the UV, if desired (improving SSKK).

**Initial Solve for  $k$ .** Lookup tables are used with user-supplied values to solve for  $k$  for each grain size spectrum. Results are plotted and all plots and parameters are downloadable (also throughout the program).

**First Global  $k$ .** Using a constant  $n$  and scalar values for phase function coefficients, this step iteratively minimizes data for all grain sizes against supplied spectra to derive a single grain-size independent  $k$ . This section delivers output values for each startpoint along with the final value of  $k$  and data fits (Figure 2).

**Combine with MIR  $k$ .** This section allows the user to upload MIR  $k$  data to obtain a more accurate SSKK transformation in the next step. There are several data combination methods available and a no-MIR data option.

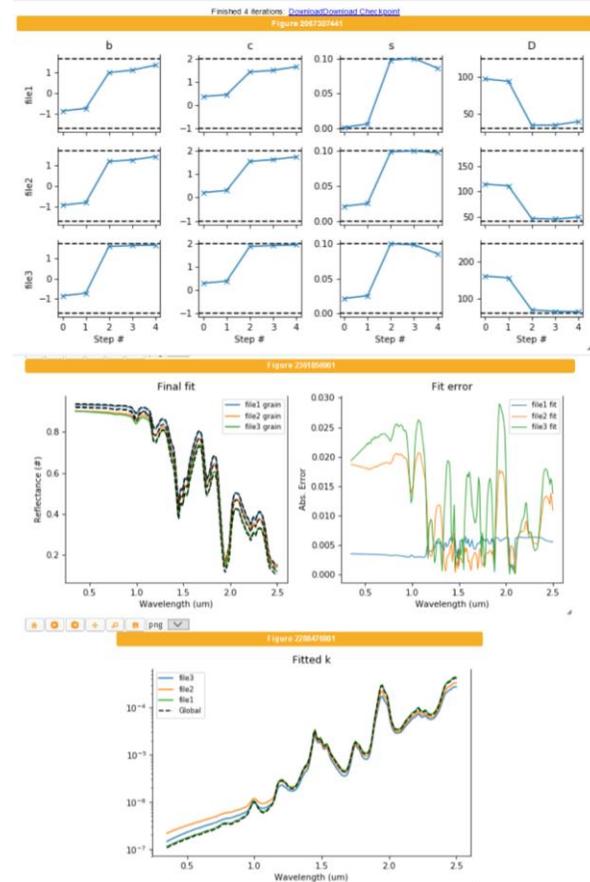
**Singly Subtractive Kramers Kronig.** The program quickly computes the VNIR  $n$  from VNIR (and MIR)  $k$ .

**Phase Function Minimization.** Here, wavelength-dependent  $n$  and  $k$  are used with optional scale and offset factors (so the solution is not overconstrained) to determine the wavelength-dependent phase function coefficients for each grain size, while optimizing  $\langle D \rangle$  and  $s$ .

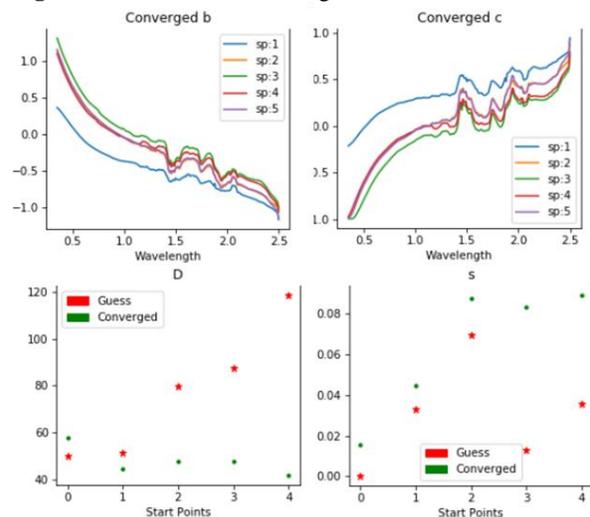
**Repeat global  $k$ .** This step takes the phase function coefficients, allowing for scaling and offset, and performs another minimization for a global, grain-size independent  $k$ . Results from this section can be downloaded and fed back in at the  $k$  combine step.

**Futue Work:** Recent redevelopment of the MatLab code has led to what appears to be a more robust data handling procedure [5]. The python code will be updated to reflect these developments in a new branch. These can be downloaded at: <https://github.com/avogadroskitty/HappyHapke>. This software can also be run natively for those who interested in adjusting theoretical or grammatical elements. The final web interface will remain at <http://opcon.mtholyoke.edu>.

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**Figure 2.** Results from the first global  $k$  minimization.



**Figure 3.** Sample plots from phase function minimization.

**References:** [1] Carey C. et al. (2017) LPS XLVII, Abstract #1097. [2] Sklute E. C. et al. (2015) *Am. Mineral.*, 100, 1110-1122. [3] Hapke, B. (2012) Cambridge University Press, UK, 507p. [4] Chandresekhhar, S. (1960) Dover, New York. [5] Sklute, E. C. et al. (2021) *52<sup>nd</sup> LPSC*, Abstract #1258.