**USING MICROSOFT EXCEL FOR HAPKE MODELING: A TECHNIQUE TO SIMPLIFY CALCULA-TIONS OF OPTICAL CONSTANTS AND REFLECTANCE SPECTRA.**

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**Introduction:** Hapke radiative transfer modeling [1,2] provides a method for determining surface composition, mineralogy, and particle size from reflectance data of fine powders [3]. If optical constants for surface components are available, remote sensing spectra can be easily and accurately analyzed. Optical constants (or complex indices of refraction) are fundamental properties of a mineral and are independent of particle size and shape. The complex index of refraction, of the form $\mathbf{n} = n\text{-}ik$ or sometimes $\mathbf{n} = n(1\text{-}ik)$, has two coefficients: $n$, the so-called real index of refraction, and $k$, the coefficient of the imaginary index of refraction [2]. The spectral features apparent in absorption or reflectance spectra of mafic minerals in the near-IR are dominated by variations in $k$, which are calculated here.

A limitation of radiative transfer modeling, however, is that optical constants for most of the major rock-forming minerals are not available, or only exist only for a few compositions. Bidirectional reflectance measurements of lunar simulant materials allow the calculation of optical constants using radiative transfer theory. Direct measurement of optical constants is infeasible for many materials because samples often have sufficient optical defects at the macroscopic level to prohibit standard transmission methods for deriving absorption coefficients. To circumvent this problem, Hapke modeling includes a method to derive optical constants from the reflectance of powders of known composition and particle size [2].

In the past, the computation of optical constants has been tied to expensive numerical analysis packages such as IDL or MATLAB. These software tools have a steep learning curve and require significant coding proficiency. A more accessible platform for the computation of optical constants is desired. To this end, the Hapke model calculations are coded into a Microsoft Excel spreadsheet. This spreadsheet is used to compute $k$ for laboratory-measured reflectance spectra of synthetic lunar glasses [3].

In many cases, calculations integrated into a spreadsheet are more manageable and easier to understand than commands in a higher-level language. Excel is much more broadly understood than IDL, and almost everyone with a computer has a copy because it is not cost-prohibitive. Interested individuals can easily investigate the structure of the spreadsheet to understand the Hapke modeling process and input their own spectra. Though Excel has limited accuracy compared to more robust mathematical programming packages, it is shown that acceptable approximations of optical constants can be produced (Fig. 1).

**Methods:** To convert bidirectional reflectance data into imaginary indices of refraction, two main steps of calculation must be undertaken. Reflectance spectra must be converted into single scattering albedo ($w$), the probability that an individual proton will be scattered by a grain. $w$ is then used to calculate $k$ [2]. Both of these steps require optimization. Our two-step method for accomplishing Hapke modeling calculations in Excel is described below.

*Single Scattering Albedo.* Calculating $w$ from input spectra requires optimization between spectra and computed radiance coefficients ($r_c$), a proxy for directly measured spectral input. The radiance coefficient is dependent on the phase angle of spectral measurements, and functions are incorporated to model components such as backscattering and offsets from isotropic behavior. Setting these values appropriately [2], the radiance coefficient is related to $w$ by the isotropic H function [2,4].

In our Excel implementation of the Hapke model, $w$ is optimized to find radiance coefficients matching input spectral data. This optimization is accomplished by referring to a table of values of $r_c$ and $w$. For accuracy, $r_c$ is calculated for 1000 values of $w$ varying stepwise from 0-1. A linear interpolation between adjacent values is conducted to improve accuracy. The VLOOKUP() function is used to find the value of $r_c$ nearest to the spectral measurement, and the corresponding single scattering albedo is output. This process is repeated for each wavelength.

*Optical Constants.* Imaginary indices of refraction ($k$) are calculated using a similar optimization process. Values of $w$ are divided by $Q_E$, the extinction efficiency ($Q_E$ =1 for closely spaced particles), to find the scattering efficiency ($Q_S$). $Q_S$ is dependent on the average grain size of the powder ($D$), wavelength of incident light ($\lambda$), the internal absorption coefficient ($s$), and both the real and imaginary indices of refraction ($n$ and $k$) of the medium. The model cannot simultaneously calculate both $n$ and $k$ to form a complete optical constant, so $n$ is estimated. For many mafic materials, $n$ is dependent on FeO content [2]. In this spreadsheet,

$n$ is calculated for synthetic lunar glasses using the formula $n = 1.644 + 0.00264 \times$ Mg# [5], where Mg number is the molar Mg/(Mg+Fe) ratio for the sample [2]. $D$ is estimated for the sample, and internal absorption is set to $s$=0 [2]. Within these constraints, $Q_S$ can be related to $k$ for each wavelength.

To convert single scattering albedo to optical constants in Excel, $k$ is derived for each wavelength using optimization. The scattering efficiency is calculated over a range of $k$ for each wavelength of the initial spectra to create a table of values. For each wavelength, the INDEX() function is used to find the largest $Q_S$ in the table of values that is smaller than $w/Q_E$. A linear interpolation between adjacent $Q_S$ values is used to find the exact optical constant. This optimization produces a $k$ value for each wavelength, thus converting the entire reflectance spectra to a range of optical constants.

*Discussion: Data input.* Spectra are input into the spreadsheet as two columns of data, one containing wavelength and the other containing the corresponding reflectance measurement. For our measurement of synthetic lunar yellow glass, the data has a spectral range from 0.5 to 2.5 μm and a resolution of 1 nm. Model variables are grouped and can be changed at will (Fig. 2). The real index of refraction, average grain size, and incidence and emission angles depend on the sample,

while the rest of the variables are generally held constant [2].

*Results.* Calculation of optical constants takes about one minute (though this is depends on the speed of the computer). The model outputs a list of $k$ by wavelength and a chart of $k$ vs. wavelength (Fig. 1).

**Conclusion**: Imaginary indices of refraction calculated using the Excel spreadsheet are similar to $k$ calculated in IDL (Fig. 1). The Excel data trends slightly downward relative to IDL values as wavelength increases. Further work will attempt to explain this systematic variation by tuning model parameters.

The analytical tools of Excel, while limited with respect to IDL or MATLAB, can yield estimates of $k$ that are similar to these higher level numerical software tools. Now that we know calculation of $k$ is possible, future work will include calculating reflectance spectra of complex mixtures given $k$ values of the component materials.

**References:** [1] Hapke, B. (1981) *JGR, 86 (B4)*, 3039-3054. [2] Lucey, P. G. (1998) *JGR, 103*, 1703-1714. [3] Gillis-Davis, J.J., et al. (2008) *LPSC 39*, CD-ROM #1535. [4] Hapke, B. (1993) Theory of reflectance and emittance spectroscopy. Cambridge Univ. Press, Cambridge, 455. [5] Wilcox, B.B., et al. (2006) *JGR, 111*, doi:10.1029/2006JE002686.
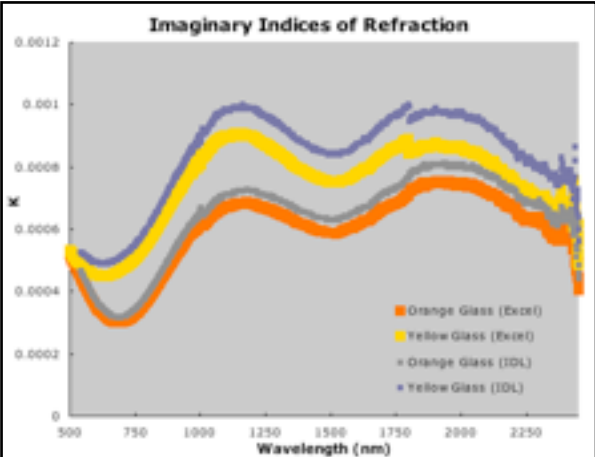


**Fig 1.** Imaginary indices of refraction for synthetic yellow and orange glasses [3] computed by IDL and Microsoft Excel.
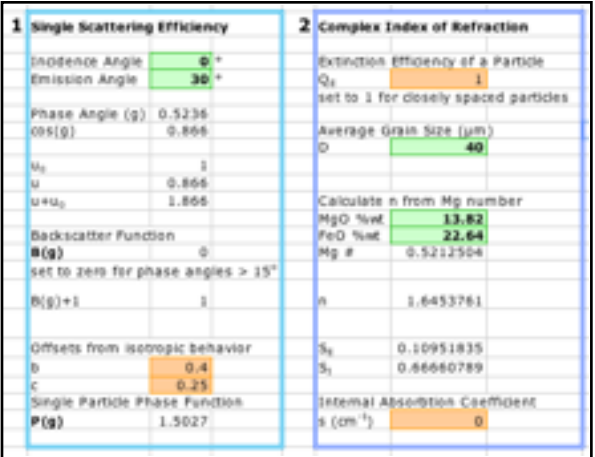


**Fig 2**. Input parameters for the Hapke modeling spreadsheet. Highlighted values are independent. Green background signifies sample-specific values, while orange shows model assumptions as described in [2].