

DECONVOLUTION OF SPECTRA FOR INTIMATE MIXTURES John F. Mustard, Carle M. Pieters and Stephen F. Pratt, Brown University, Providence, RI 02912.

Visible to near-infrared reflectance spectra of macroscopic mixtures have been shown to be linear combinations of the reflectances of the pure mineral components in the mixture (1). However, for microscopic or intimate mixtures the mixing systematics are in general non-linear (2,3). The systematics may be linearized by conversion of reflectance to single-scattering albedo ( $w$ ), where the equations which relate reflectance to  $w$  depend on the method of data collection (bihemispherical, directional hemispherical, or bi-directional reflectance) (4). Several recently proposed mixing models may be used to estimate mineral abundances from the reflectance spectra of intimate mixtures. These models are summarized below and a revised model is presented.

Johnson *et al* (5) present a semi-empirical mixing model based on the work of Hapke (4). They used directional-hemispherical reflectance data measured in the laboratory and combined pure mineral spectra to fit the spectrum of a mixture using an iterative least squares approach. Although the fits of endmember spectra to mixture spectra were within experimental error, the predictions of mineral abundances were 2% to 30% from the actual values. A more recent approach has been to apply principal components analysis (PCA) to collections of laboratory and lunar spectral data measured as or, converted to directional-hemispherical reflectance (6,7). This technique may be used to determine the type of mixing (macroscopic *vs.* intimate), identify the potential endmembers from a suite of spectra and estimate the relative proportions of endmembers in a sample. The advantages of PCA are the identification of endmembers with limited *a priori* knowledge and approximate mixing relations between endmembers. The disadvantages are that it requires careful interpretation of the principal axis of variation and the quantitative determination of endmember abundances becomes complex for mixtures containing more than two components.

We have used a similar curve fitting approach as Johnson *et al* (5) with the following exceptions. We use a non-iterative (*i.e.* linear) least squares approach and the data, measured as bi-directional reflectance with incidence and emergence angles of  $30^\circ$  and  $0^\circ$  were converted to  $w$  by the following simplified version of Hapke's (4) equation for bi-directional reflectance

$$r(i,e) = \frac{w}{4(\mu + \mu_0)} (2.2 + H(\mu)H(\mu_0)) \quad H(\mu) = \frac{1+2\mu}{1+2\mu\gamma} \quad (1)$$

where  $r$  is the measured reflectance,  $i$  is the incidence angle,  $e$  is the emergence angle  $\mu = \cos(e)$ ,  $\mu_0 = \cos(i)$  and  $\gamma = (1-w)^{-1/2}$ . Hapke (4) predicts that for intimate mixtures, the mean single-scattering albedo is related to the single-scattering albedo of each of the components by

$$w(\lambda) = \left( \sum_i w_i(\lambda) M_i p_i d_i \right) / \left( \sum_i M_i p_i d_i \right) \quad (2)$$

where  $M_i$ ,  $p_i$ , and  $d_i$  are the mass fraction, density and mean particle diameter of each of the  $i$ -components in the mixture. The endmember mineral spectra were combined to fit the measured mixture spectra by a single least squares inversion of equation (2). The fractional contribution of each endmember is given by the relative geometrical cross section ( $f$ ) where  $f_j = (M_j/p_j d_j) / (\sum_n M_n/p_n d_n)$  for the  $j$ th component of an  $n$ -component mixture.

This model was tested with two mixture series composed of 45-75  $\mu$ m particles: an anorthite-enstatite series (two minerals of similar overall albedo) and an olivine-magnetite series (two minerals with strongly different overall albedos). The quality of the least squares fits as determined by the standard deviation are not greater than  $5 \times 10^{-3}$  in all cases. The standard deviation is determined by curve shape only and is not sensitive to the effects of sample preparation which may result in up to a 2% offset in the measured reflectance curves (5). Shown in Fig. 1 are the observed and least squares fit spectra for the anorthite-enstatite mixture series.

The computed and actual values for  $f$  are shown in Figs. 2 and 3. It is evident from Fig. 2 that, for mixtures of comparable albedo, equations (1) and (2) can be used to predict the known fractional abundances to within the experimental error. This degree of accuracy is more than sufficient for the purposes of estimating surface mineral abundances from known or assumed endmembers. The simplified version of Hapke's (4) equation is less satisfactory for mixtures containing low albedo materials as shown in Fig. 3. The model consistently overpredicts the olivine content and underpredicts the magnetite abundance. The systematic deviation of computed from actual values of  $f$  for the mixtures containing low albedo minerals suggests that either a more rigorous treatment of Hapke's (4) equations is needed or an empirical adjustment to equation (1) will allow a more accurate solution to be developed.

These data indicate that the simplified version of Hapke's equation for bi-directional reflectance (equation (1)) may be used to deconvolve reflectance spectra into mineral abundances if appropriate endmembers are known or derived from other techniques. For surfaces that contain a significant component of very low albedo material, a somewhat modified version of this technique will need to be developed. Due to the nature of equation (2) above, this model can also be easily expanded for use with multicomponent mixtures. Since the abundances are calculated using a non-iterative approach, the application of this method is especially efficient for large spectral data sets, such as those produced by mapping spectrometers (NIMS, AVIRIS, etc.)

References: (1) Singer, R.B., and McCord, T.B. (1979) *Proc. Lunar Planet. Sci. Conf. 10th.* 1835-1848. (2) Nash, D.B., and Conel, J.E. (1974) *J. Geophys. Res.* **79**, 1615-1621. (3) Singer, R.B. (1981) *J. Geophys. Res.* **86**, 7967-7982. (4) Hapke, B. (1981) *J. Geophys. Res.* **86**, 3039-3054. (5) Johnson, P.E., Smith, M.O., Taylor-George, S., and Adams, J.B. (1983) *J. Geophys. Res.* **88**, 3557-3561. (6) Smith, M.O., Johnson, P.E., and Adams, J.B. (1985) *J. Geophys. Res.* **90**, C797-C804. (7) Johnson, P.E., Smith, M.O., and Adams, J.B. (1985) *J. Geophys. Res.* **90**, C805-C810.

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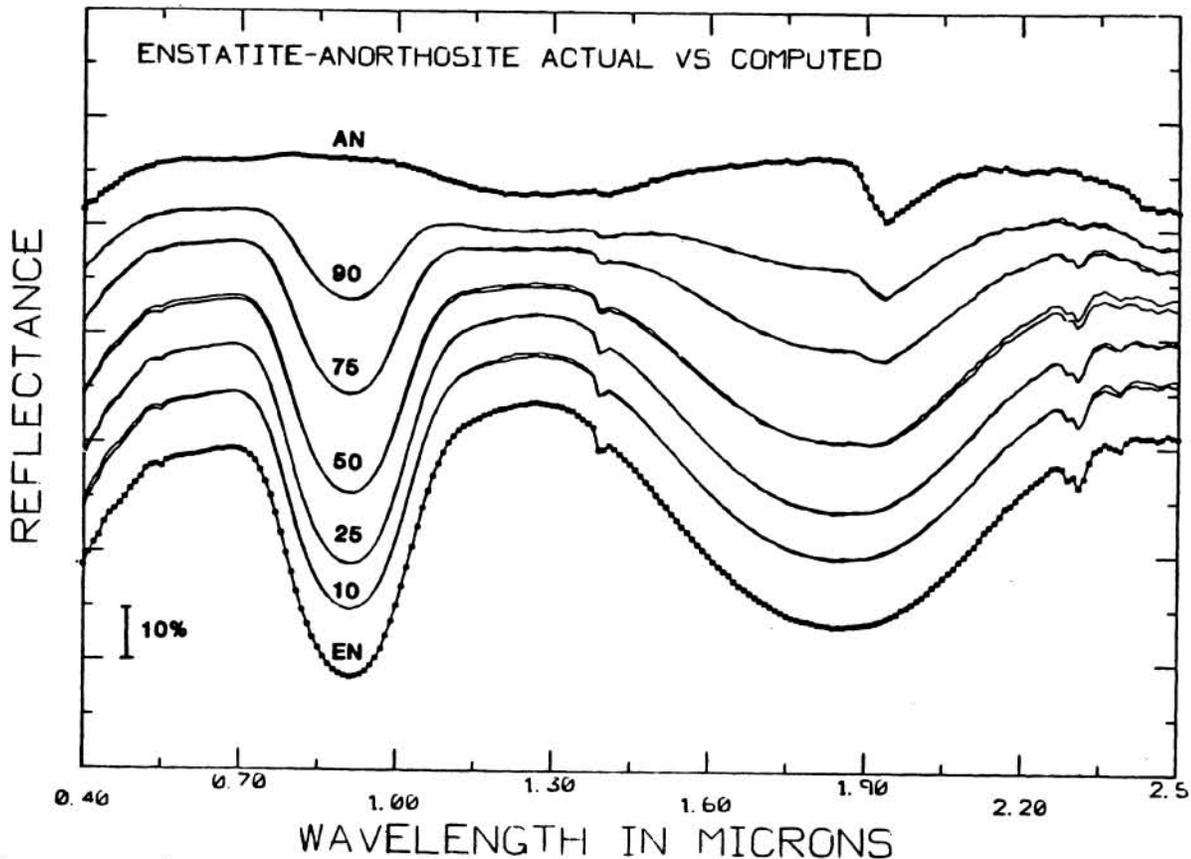


Figure 1. Actual and calculated bi-directional reflectance spectra for the anorthite-enstatite mixture series. The dotted curves, labelled AN for anorthite and EN for enstatite, are the endmember spectra used to model the mixture spectra. The smooth curves are the actual and calculated spectra plotted together. The number located in the 0.9  $\mu$ m. absorption band corresponds to the % mass of anorthite in the mixture. Each pair of calculated and actual spectra are offset for clarity and to emphasize the quality of the curve fits. At this scale there is almost no difference between the calculated and actual spectra.

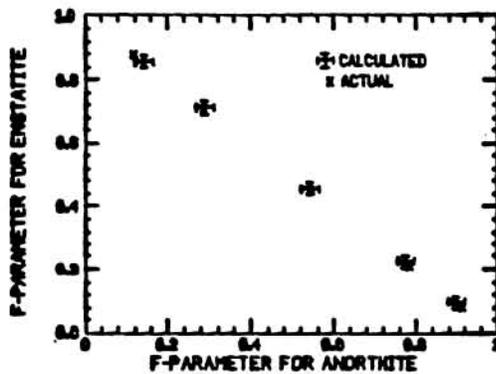


Figure 2. Actual and calculated relative geometrical cross sections (f-parameters) of anorthite and enstatite plotted against one another for the mixture series shown in Fig. 1. The calculated values are obtained from the curve fitting technique described in the abstract. The calculated values are generally within 1.5% of the actual values which is adequate for estimating mineral abundances in the mixtures.

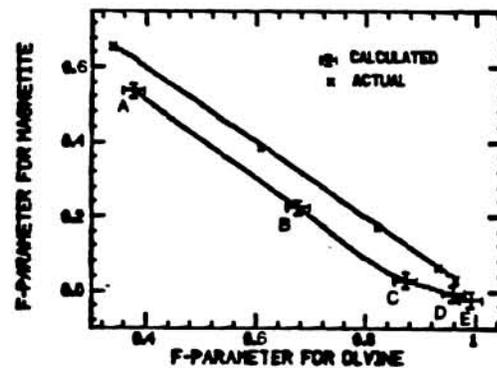


Figure 3. This is the same type of plot as in Fig 2 for the olivine-magnetite mixture series. The letters correspond to the mass fraction ratios where A=25/75, B=50/50, C=75/25, D=90/10, E=95/5, and the first number is the % mass of olivine in the mixtures. The lines between data points were added to emphasize the systematic overprediction of olivine content and underprediction of magnetite content.