

**REFLECTANCE SPECTRA OF FIVE-COMPONENT MINERAL MIXTURES:  
IMPLICATIONS FOR MIXTURE MODELING** S. G. Herzog and J. F. Mustard, Department of Geological Sciences, Brown University, Providence, RI 02912

The surfaces of the terrestrial planets consist largely of particulate materials, or soils, whose compositions and particle size distributions are products of geologic processes. The reflectance spectrum of a particulate surface represents a systematic combination of the mineralogy and particle size distribution of the material. Both composition and grain size information are useful in geologic interpretation of a surface, but are convolved in a single reflectance spectrum. We used spectral mixture analysis to separate these parameters by modeling the reflectance of five-component laboratory soils which vary in grain size. We find that successful prediction of endmember compositions requires some knowledge of grain size distribution, and that the fine particles dominate the mixed spectrum in excess of volume fraction and intimate mixture model predictions.

The effects of mineral composition and particle size on reflectance spectra are reasonably well understood for single grains and homogeneous materials. Compositional information is obtained from diagnostic spectral absorption features of minerals [1, 2]. For a given chemical composition, in the visible to near-infrared wavelength region, small particles yield brighter reflectances, and have weaker absorption bands than spectra of larger particles.

Hapke [5] has developed a model of bidirectional reflectance for particulate materials which can be used to determine the relative proportions of components in a particulate mixture. The mixing systematics of fine particulate materials are non-linear because of multiple photon interactions. If the particles are assumed to have similar shapes and the particle diameters are much greater than the wavelength of light, then the mixing systematics can be linearized by converting the reflectance data to single-scattering albedo (SSA). The SSA is predicted to be a linear mixture of the SSAs of the endmembers weighted by their relative geometric cross-sections [5]. A simplified approach to this model suitable for application to remotely acquired data requires some assumptions regarding phase angle and effective grain size, but has been demonstrated to yield endmember abundances with an accuracy of about 5% if the reflectance spectra of the endmember components themselves are known [6, 7, 8]. However, these applications have generally been confined to narrow particle size separates that are not realistic representations of natural particle size distributions, and have not examined mixing of more than three minerals. For the SSA spectrum of each mixture the model predicts a combination of endmember SSA spectra from among the available endmembers which best fits the mixture spectrum in a least squares sense. The combination which yields the minimum standard deviation from the observed spectrum is predicted to represent the quantities of endmembers in the mixture. Geometric cross-sections of the predicted components are converted to mass fraction by using a priori information or making assumptions about particle size and mineral composition. We used this model to predict the quantities of specified endmembers in the mixtures with the principal goal of separating composition and grain size as mixture endmember properties.

**Experimental Procedure:** The five principal minerals which comprise the basaltic and gabbroic rocks were used in these experiments: clinopyroxene; orthopyroxene; olivine; plagioclase; and ilmenite (a proxy for opaques). Each of these minerals was crushed and wet-sieved to three particle sizes: <25  $\mu\text{m}$  (small); 25-75  $\mu\text{m}$  (medium); and 75-250  $\mu\text{m}$  (large). The particle size separates were combined to make monomineralic soils in the following proportions - small soil (SS): 65 weight percent small separate, 25 % medium, and 10% large; medium soil (MS): 25 % small, 50% medium, 25 % large; and large soil (LS): 10% small, 25 % medium, and 65% large separate. A total of six grain size groups are thus available for each mineral composition. Polyminerallc soils which represent disaggregated equivalents of four types of gabbroic rocks were then constructed in five different compositions and three different grain size distributions, each of which contains a controlled distribution of the three particle size separates. The soil compositions and grain size groups are shown in Table 1. The visible to near-infrared reflectances of all particle size separates, monomineralic soils, and gabbroic soils were measured in RELAB, with a wavelength range of 300 to 2600 nm. The monomineralic size fractions and soils spectra were previously reported in [3, 4].

We first modeled the spectra of the monomineralic soils using the three grain size separates as endmembers, to predict particle size for a given composition. The predicted mass fractions were generally within 0.2 of the actual abundances. The monomineralic spectra were then modeled using only the small and large fractions as possible endmembers. This test requires the fraction of the medium separate to be divided between the small and large fractions for comparison with model-predicted values. Standard deviations of the predicted values were again low, but predicted fractions varied more from the calculated values. The fine grain size separate was invariably predicted by the model to account for most of the mass of the individual soils.

The fractions of correct grain size endmembers for the synthetic gabbroic soils were then modeled to determine the effectiveness of interpreting composition if the correct grain size distributions are given. Figure 1 illustrates the correct endmember fractions and the fractions predicted by the model for three grain size distributions for each composition. Solid symbols indicate the actual mass fractions used in the mixed soils, and hollow symbols indicate the mass fractions predicted by the intimate mixture model. Only the high-Ti mare basalt and the gabbroic anorthosite show negative fractions of some endmembers. For all four compositions, the medium size fraction (group A) is the most accurately predicted for most compositional endmembers, and in general the small soil fraction caused the greatest error in predicted quantities.

**Discussion:** This study is the first to model spectral reflectance of five-component mixtures with wide grain-size distributions. The intimate mixture approach of Hapke [5] contains a limitation in that the relative geometric cross-section of a material assumes an effective grain size, which is an approximation to an actual range of grain sizes, and must be selected a priori in order to model compositions. Normally this information is not available for interpretation

of remotely obtained spectra. There is a theoretical endmember grain size (large) above which absorption features cease to strengthen with increasing grain size (saturation). There should likewise be a theoretical grain size endmember (small) beyond which reflectance ceases to increase with decreasing grain size. This is intuitively correct because characteristic mineral spectra are not observed to disappear at small particle diameters. All the materials under study consist of some combination of three different grain size fractions. However, our results indicate that reflectance spectra of mixtures of several grain sizes is not predicted by the intimate mixture model. Rather, the fine fraction dominates the mixed spectra. Fine particles have brighter reflections and weaker absorptions, and may accurately model the reduced spectral contrast of the mixtures without requiring significant contribution of the large grain sizes.

An interesting trend manifested in almost all the model results is the error in the predicted fractions of olivine and ilmenite components in the mixtures. These may be due to the similarity of the olivine spectra to a combination of the other spectra; and because ilmenite has a flat, dark reflectance which the model incorporates to decrease the reflectance of the other components. Use of increased numbers of endmembers may result in increased similarity between spectra, and thus a decrease in the ability of the model to resolve different endmembers.

The principal result manifested in all the modeled spectra is the overwhelming effect of fine particles on the mixed spectra. Small particle size materials have bright reflectance and weak absorptions, and when mixed with other particle sizes, dominate the mixed spectrum in excess of their volume proportions, and in excess of the model prediction. These results indicate that successful modeling may require greater emphasis to be placed on the fine fraction of particulate mixtures, and we are pursuing this possibility.

References: [1] Burns R. G. (1970) *Mineral. Appl. Crystal Field Theory*. [2] Hapke, B. (1981) *JGR* 86: 3039; [3] Johnson P. E. et al. (1983) *JGR* 88: 3557; [4] Mustard J. F. and Pieters C. M. (1987) *Proc. LPSC 17th*; [5] Mustard J. F. and Pieters C. M. (1989) *JGR* 94: 13619; [6] Mustard et al. (1993) *LPSC 24*; [7] Pieters et al. (1993) *LPSC 24*

Table 1

Compositions and Grain Sizes of the Synthetic Soil Mixtures

	Tholeiite		Low-Ca Basalt		High-Ti Mare		Gabbroic Anorth.		Group A	Group B	Group C
	Vi	Xi	Vi	Xi	Vi	Xi	Vi	Xi	med cpx	MS cpx	FS cpx
cpx	0.40	0.42	0.10	0.10	0.50	0.47	0.20	0.23	med. opx	MS opx	FS opx
opx	0.10	0.11	0.50	0.49	0.05	0.05	0.00	0.00	med. olv	MS olv	FS olv
olv	0.20	0.21	0.30	0.30	0.05	0.05	0.00	0.00	med. alb	FS alb	MS alb
alb	0.28	0.23	0.05	0.04	0.20	0.15	0.75	0.69	med. ilm	MS ilm	MS ilm
ilm	0.02	0.03	0.05	0.07	0.20	0.28	0.05	0.08			

Vi : volume fraction; Xi : mass fraction      med: 25-75 um; MS: 25:50:25 s:m:l; FS: 65:25:10 s:m:l

Figure 1

