MODELLING OF MINERAL MIXTURE REFLECTANCE SPECTRA. F. Poulet, S. Erard, A. Gendrin, *IAS, Universite Paris-Sud, 91405 ORSAY Cedex, France (francois.poulet@ias.fr).*

Introduction

In the forthcoming years, high spectral resolution imaging spectroscopy in the visible/near-infrared range will be used to obtain compositional information for planetary surfaces (especially for Mars surface with the space missions Mars Express and Mars Reconnaissance Orbiter). Deconvolving a reflectance spectrum to mineral abundance in an umabiguous way is difficult, because the spectra are complex nonlinear functions of grain size, abundance, material opacity, and type of mixtures (dust, sand, areal).

The common approach is to extract information from the measured spectrum itself, using e.g. the Modified Gaussian Model [1] or automated band detection [10]. The strength of these methods is to aid in determining appropriate endmembers to model, but no information can be derived on abundance, grain size, and type of mixtures of the end-members.

Multiple scattering models can provide approximate solutions to the radiative transfer in a particulate medium. One such model is the semiempirical Hapke model [2] which has been used by most modelers of natural and laboratory common geologic mixtures. Applications of the Hapke model to quantitative analysis of laboratory mineral intimate mixtures give abundances estimates better than 10% if an estimate of the particle sizes of the respective mixture components is known [3,4].

A geometrical optics model for albedo spectral dependence of regolith-like surfaces was presented by Skhuratov et al. [5]. The purpose of the paper is to use the Shkuratov scattering theory to determine the type of mixture, the relative proportions, and the grain sizes of components (minerals) of laboratory common geologic mineral mixtures given reflectance spectra of the endmembers only.

Modelling method

The formulation of the Shkuratov model can be summarized into three steps: 1) to derive the albedo of a particle of given composition (defined by the optical constants $n(\lambda)$, $k(\lambda)$) and size d; 2) to derive the reflectance of an homogeneous and single-member particulate surface; 3) to derive the reflectance of a certain type of mixture. Here, two kinds of mixtures are considered: intimate (or "salt-and-pepper") mixture of coarse particles of size $\gg \lambda$ and areal mixture (or "checkerboard"). Note that mixture of particles of size $\ll \lambda$ (dust mixture) can be in principle constructed from the Shkuratov theory. In terms of formulation, the main difference between the Hapke and the Shkuratov theory is the role of the phase function of individual particles, which is automatically calculated (and generally forward directed) in the case of the Shkuratov model instead being a free parameter (but effectively dominated by isotropic scattering) as formulated in the Hapke model [6]. Shkuratov theory incorporates realistic grain forward scattering at all orders of scattering, while most applications of Hapke theory include it only to first order.

One of strengths of the Shkuratov theory is that the model is analytically invertible: the imaginary index fraction $k(\lambda)$ can be found if the spectral albedo is known and estimates for n and d are available.

Our procedure of deconvolution is first to calculate k from each endmember spectrum; we then use the scheme described above to reproduce the mixture spectra by optimizing the type of mixture (intimate or areal), the grain sizes and the abundances of endmembers.

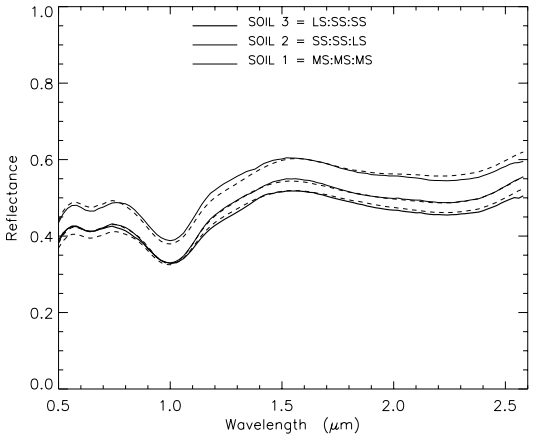

Figure 1: Reflectance spectra of gabbroic rocks (continuous line) compared to their best-fit spectra (dashed line).

Modelling results

Shown in Table 1 are the optimized parameters for intimate clinopyroxene(CPX)/orthopyroxene(OPX) mixtures [7]. Both intimate and areal mixtures are considered. The noticeable differences in terms of RMS and abundance between the areal and intimate mixtures allow to reject areal mixture as a possible mixture solution. Modellings of five intimate pyroxene mixtures (0/1,0.25/0.75,0.5/0.5,0.75/0.25,1/0) for three grain sizes (0-45, 45-75, 75-125 μm) demonstrate that the method is valid for deriving accurate estimates of the abundances of minerals to within 8% AND grain sizes within a factor 2.

Further tests are done in using the complex mixtures described by [8]: three minerals (CPX, OPX and OLIvine) were sieved to three particle sizes (<25 (S), 25-75 (M), 75-250 (L) μm). Particle size separates were combined to form monomineralic soils in the following proportions: small soil (SS = 65% S 25% M 10% L), medium soil (MS = 25% S 50% M 25% L), and large soil (LS = 10% S 25% M 65% L). Monomineralic soils were combined with a constant mass fraction ratio of 3:1:1, similar to mafic mineral ratios in gabbroic rocks with three different soil combinations: SOIL 1 = MS:MS:MS, SOIL 2 = SS:SS:LS, SOIL 3= LS:SS:SS. Therefore, the soils are the combination of 9 components (3 grain size separates for each mineral). To limit the number of parameters, we have chosen to model the soils by an intimate mixture of 6 compo-

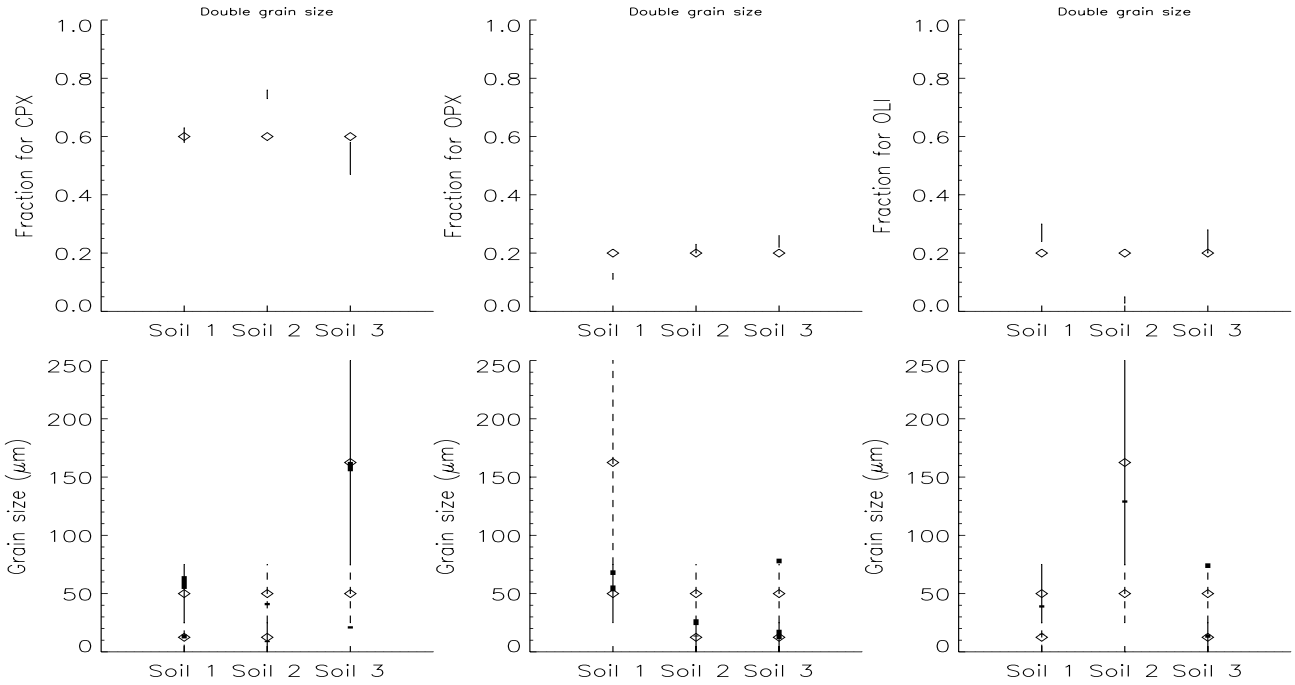

Figure 2: Calculated proportions (top, solid lines) and grain sizes (bottom, thick lines) of each endmember for the three grabboic soils. The actual half-size and half-fraction are shown by lozanges. In bottom figures, the thin and dashed lines define the intervals of actual sizes of the two largest components in term of abundance.

Table 1: Optimized parameters for enstatite (OPX) and clinopyroxene (CPX) intimate mixtures. The particle size range is 75-125 μm (half-size=100 μm). Two types of mixture are considered.

ENDMEMBERS	Actual abundance	Type of mixture	Computed Abundance	Computed Grain Size (μm)	RMS (%)
OPX/CPX	0.75/0.25	Intimate	[0.73,0.75]/[0.25,0.27]	[93,101]/[203,256]	0.4
OPX/CPX	0.75/0.25	Areal	[0.47,0.52]/[0.48,0.53]	[62,74]/[130,160]	1.3
OPX/CPX	0.50/0.50	Intimate	[0.44,0.46]/[0.54,0.56]	[90,100]/[129,141]	0.3
OPX/CPX	0.50/0.50	Areal	[0.29,0.36]/[0.71,0.64]	[70,105]/[130,160]	1.2
OPX/CPX	1/0	Intimate	[0.99,1]/[0,0.01]	[103,105]/[103,104]	0.02
OPX/CPX	0/1	Intimate	0/1	–/[100,102]	0.02

nents: a double grain sizes for the three endmember, which leads to optimize a total number of 12 parameters (2 grain sizes and 2 fractions for each component). Shown in Fig. 1 are best-fit reflectance spectra compared to the measured spectra of three soils. The actual grain sizes and fractional abundance of components in the three soils calculated using the simplex approach are presented in Fig. 2. This figure allows a rapid qualitative assesment of the accuracy of the fits. The derived fractions agree with the actual values to within 10% for most, and within 15% for all components. Grain sizes of all end-members are calculated to within the intervals of actual grain sizes.

These results indicate that the method presented can be used to accurately estimate the relative proportions of components as well as the grain sizes. The type of mixture (areal, intimate, dust) can also be tested. This method has proven to be a very useful tool and can provide good estimates of surface abundance of minerals from mixed surfaces. This deconvolution method is used to investigate the surface composition of low albedo regions from ISM spectra in a companion abstract [9]. It will also be included in the data processing scheme for OMEGA onboard Mars-Express.

Reference [1] Sunshine, J. M. et al. (1990) *JGR*, 95, 6955-6966. [2] Hapke, B. (1981) *JGR*, 86, 3039–3054. [3] Mustard J.F. and Pieters C.M (1987), *JGR* 92, E617–E626. [4] Mustard J.F. and Pieters C.M (1989), *JGR* 94, 13619–13634. [5] Shkuratov et al. (1999) *Icarus* 137, 235–246. [6] Poulet F. et al. (2002) *Icarus* 160, 313–324. [7] Sunshine J.M. and C.M. Pieters (1993), *JGR* 98, 9075–9087. [8] Pieters C.M. et al. (1993) *LPSC* XXIV, 1147-1148. [9] Poulet F. et al. (2003) *LPSC* XXXIV. [10] Gendrin A. and Erard S. (2003) *LPSC* XXXIV.