ESTIMATING MODAL MINERALOGY OF MIXTURES WITH PHYLLOSILICATES USING RADIATIVE TRANSFER MODELING OF VISIBLE/NEAR INFRARED SPECTRA. B. L. Ehlmann[1], J. F. Mustard[2], F. Poulet[1] , T. Hiroi[2]. [1]Institut d'Astrophysique Spatiale, Université Paris-Sud (bethany.ehlmann@ias.u-psud.fr) [2]Dept. of Geological Sciences, Brown University

Introduction: Diverse phyllosilicates identified on Mars from visible near infrared (VNIR) spectral data from the CRISM and OMEGA instruments indicate past environments with long-lived water-rock interaction [1-3]. Qualitative mineral identification and mapping permits identification of the deposits' geologic setting. However, to best constrain the extent and environment of aqueous alteration, quantitative estimates of mineralogic composition, i.e. abundance of hydrated phases and surface modal mineralogy, are essential. Here we investigate the accuracy of VNIR radiative transfer modeling for quantitative mineralogy using a suite of prepared mineral mixtures.

Linear deconvolution of thermal emission data permits volumetric abundances of coarse grain size mineral constituents in surface units to be determined to within 5-15% [e.g. 4-6] because the photon interactions are mostly singly scattered. In VNIR spectral data of particulate surfaces, multiple scattering dominates and spectral mixing is nonlinear. Laboratory studies have shown the Hapke [7-9] and Shkuratov [10,11] radiative transfer models predict modal abundance to within approximately 10% for well-controlled mixtures of mafic minerals. Applications of radiative transfer models to lunar remotely sensed data show that a more accurate understanding of geologic processes is gained relative to linear mixture models [12]. For Mars data, the Shkuratov model has been applied to estimate mineral abundances within phyllosilicate-bearing terrains using OMEGA data [13], providing a first comparison of variations in modal mineralogy.

The performance of Hapke and Shkuratov models for determining phyllosilicate abundance in mixtures has not yet been evaluated using laboratory data, however. Because of the considerable compositional variability of phyllosilicates and changes in spectral properties related to hydration state, these alteration minerals may prove more challenging to model than mafic minerals. We have measured reflectance spectra of a suite of mixtures to assess the efficacy of both the Shkuratov and Hapke models in estimating modal mineralogy of phyllosilicate-bearing assemblages.

Materials and Methods: We made mixtures that permitted testing radiative transfer models with materials of different optical and spectral properties and that were also plausible compositions found on the surfaces of planetary bodies (e.g. Mars, asteroids). The phyllosilicate used was NG-1, a well-characterized nontronite (Fe-smectite) obtained from the Clay Mineral Society and chosen because Fe/Mg smectites are the most common phyllosilicate found on Mars [1,2]. The nontronite was mixed with olivine (from the San Carlos formation); anhydrous basaltic glass (from the Big Island, Hawaii [6]), basalt (from Medicine Lake, Oregon [6]), and magnesite (Mg-carbonate; Ward's mineral supply) in binary and ternary mixtures (Table 1). Hence, phyllosilicate is mixed with bright and dark endmembers, a heterogeneous dark endmember (which itself can be modeled as multiple components), and another alteration mineral. The mafic components have broad electronic absorptions while the carbonate and clay have sharp vibrational absorptions (Fig. 1).

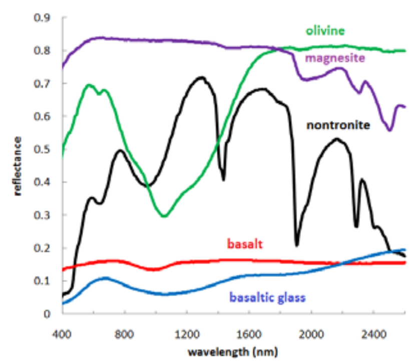

Figure 1. Reflectance spectra of endmembers, 45-75 μm particle size.

Table 1. Prepared mixture suites. All suites were prepared with 45-75 μm size fractions for each constituent. For select samples, mixtures were prepared with different particle sizes for each component. (*the basalt sample can be treated as a single component or as 5-components (plag., opx, cpx, olv. glass) since its modal mineralogy is known from [6])

Binary	**Multi-Size**
nontronite-olivine	Y
nontronite-basaltic glass	
nontronite-basalt*	Y
olivine-basaltic glass	
nontronite-magnesite	
Ternary	
nontronite-olivine-basaltic glass	
nontronite-magnesite-olivine	Y
nontronite-magnesite-basalt glass	

Each endmember was crushed and sieved into eight particle size fractions. Nontronite was dry sieved while other components were wet sieved. Reflectance spectra were measured in the RELAB bidirectional spectrometer at i=30º, e=0º. Optical constants were estimated by using the Shkuratov model to iteratively determine the imaginary index, *k*, for each endmember from reflectance spectra of the endmember particle size separates

[11, 14]. Each endmember was weighed and then mixed, resulting in suites of mixtures (containing 5 wt. %, 10%, 30%, 50%, 70%, and 90% nontronite for binary mixtures; 16%, 33%, 42%, 68% nontronite for ternary mixtures).

Results: Model estimates of nontronite abundance in binary mixture with mafic endmembers are accurate to <10% in most cases for the both Hapke and Shkuratov modeling and RMS error is <0.01 [15]. Initial Shkuratov modeling performed with an AMOEBA optimization routine exhibited a substantial sensitivity to the choice of optical constants. (Hapke modeling is currently implemented using least squares mixing based on conversion of reflectance to single-scattering albedo and does not utilize optical constants).

For ternary mixtures, model results to date show moderate agreement with actual data. For example, for mixtures of nontronite, olivine, and basaltic glass (e.g. Fig. 3), Hapke modeled modal mineralogy was within 10% of actual for 4 of the 7 mixtures. There was a systematic underestimation of the quantity of olivine present (Fig. 2a). This was insensitive to the wavelength range used. Data shown are for model runs over 1350-2550 nm, which do not consider the broad 1000 nm olivine absorption, but data from 600-2550 nm yield similar underestimations. For the Shkuratov modeling, different sets of endmember optical constants and permitted variation in grain size were tested. Modeled modal mineralogy is within 10% of actual for 5 of 7 mixtures (Fig. 2b). Shkuratov modeled data do not show systematic underestimates of a particular mineral, although grain size estimates rarely agree with the sieved size fraction (Fig. 2c) (it may be that the s, path length, parameter in the Shkuratov model is not a true proxy for grain size).

Initial results are encouraging: for binary mixtures at all abundances of hydrated minerals and ternary mixtures with hydrated minerals at high (>65%) or low (<20%) abundance, estimates of modal mineralogy are accurate to within 10%. The models appear to have more difficulty when endmember proportions are approximately equal. Our future work will look for trends in Hapke and Shkuratov model accuracy with spectral properties of mixture constituents as well as conduct sensitivity analyses on the influence of optical constants used, wavelength range considered, and optimization algorithm employed.

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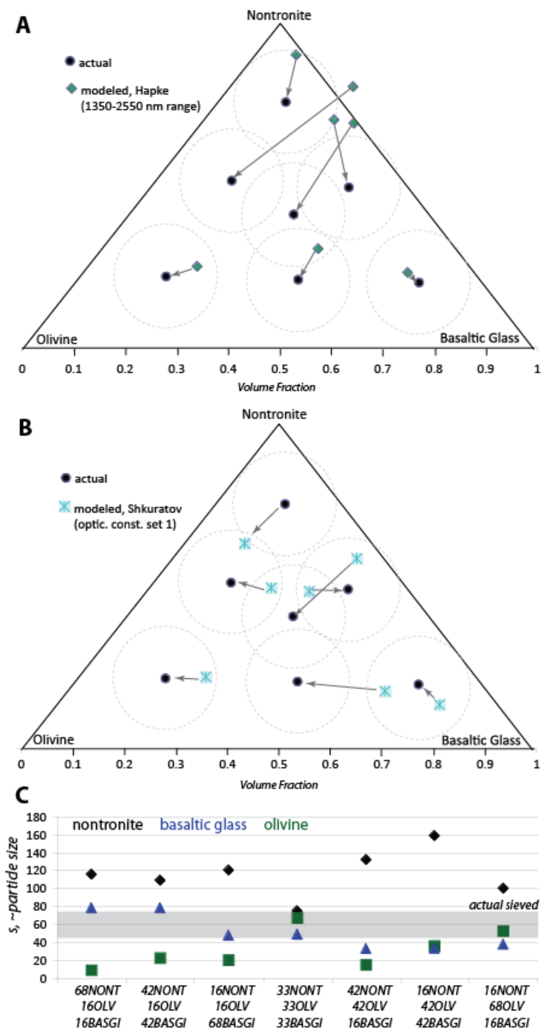
References: [1] Poulet F. et al. (2005) *Nature*, *438*, 623-627 [2] Mustard, J.F. et al. (2008) *Nature 454, 305-309* [3] Murchie, S.L. et al., (2009) *JGR*, E00D07 [4] Ramsey, M. and P.R. Christensen (1998) *JGR* 103, 577-596. [5] Feely, K.C. and P.R. Christensen (1999) *JGR* 104, 24,195-24,210. [6] Wyatt M.B. et al. (2001) JGR 106, 14,711-14,732. [7] Hapke B. (1993) *Theory of reflectance and emittance spectroscopy*. Cambridge Univ. Press. [8] Clark, R. (1983) *JGR* 88, 10,635-10,644. [9] Mustard, J.F. and C.M. Pieters, *JGR* 94, 13,619-13,634 [10] Shkuratov Y. et al. (1999) *Icarus*, *137*, 235-246. [11] Poulet F. and S. Erard (2004) *JGR*, *109*, E02009. [12] Mustard et al. (1998) *JGR* 103(E8), 19419-19425 [13] Poulet et al., 2008 *A&A* 487, L41–L44. [14] Roush, T.L. et al. (2007) *JGR* 112, E10003. [15] Ehlmann, B.L. et al. (2009) *LPSC*, abs 1771.

Figure 2. Volumetric abundances from model runs with (a) Hapke least squares modeling with endmember reflectances converted to single scattering albedo and (b) Shkuratov modeling with a narrow allowed grain size tolerance and using optical constants derived from all 8 endmembers. Values of the parameter s, an approximate proxy for particle size are shown in (c) for the Shkuratov model run. Modeled volumetric abundances were compared to actual volumetric abundances by converting from wt. % values using densities of 2.25 g/cm^3 for nontronite, 2.75 g/cm^3 for basaltic glass, and 3.3 g/cm^3 for olivine. Circles indicate ±10% compositional range.



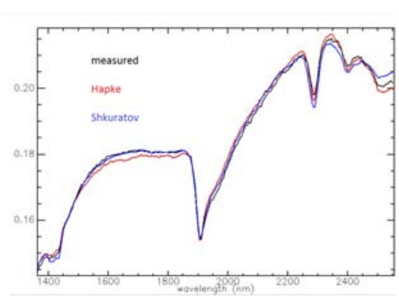


Figure 3. Example modeled and measured spectra for the sample with 16% olivine, 68% basaltic glass, 16% nontronite. RMS error is 0.002 for the Hapke fit and 0.001 for the Shkuratov fit.