

SPECTRAL UNMIXING OF CRISM HYPERSPECTRAL DATA OVER SOUTHWEST MELAS CHASMA, MARS. Y. Liu¹, T. D. Glotch², N. A. Scudder², M. L. Kraner², T. Condu², R. E. Arvidson³, E. A. Guinness³, M. J. Wolff⁴, and M. D. Smith⁵, ¹Southwest Research Institute, San Antonio, TX (yang.liu@swri.edu), ²Department of Geosciences, Stony Brook University, Stony Brook, NY, ³Department of Earth and Planetary Sciences, Washington University in St. Louis, St. Louis, MO, ⁴Space Science Institute, Boulder, CO, ⁵NASA Goddard Spaceflight Center, Greenbelt, MD.

Introduction: One important aspect of planetary remote sensing analyses is spectroscopic mineral identification and quantification on the surfaces of the terrestrial bodies. By analyzing the diagnostic features of reflectance spectra in the visible and near infrared (VNIR; $\sim 0.4\text{--}3\ \mu\text{m}$) region and the thermal emission spectra in the thermal infrared (TIR; $\sim 3\text{--}50\ \mu\text{m}$) region, we can extract valuable mineralogical information. However, the measured signal from the remote sensor always results from the interaction of photons with multiple constituents within each pixel [1]. While multispectral sensing has largely succeeded at classifying whole pixels, image interpretation issues exist as the mixed nature of the spectral information considerably constrains the accuracy of spectral analysis [2-4]. With the significant increase of spectral range and resolution in modern hyperspectral data, we are now in a position to extract and investigate detailed information about the mineral properties of pixels in a remotely sensed scene. This can be done by spectral unmixing, a quantitative analysis procedure that decomposes the measured spectrum of a mixed pixel into a collection of constituent spectra (or end-members) and a set of corresponding fractions (or abundances).

Orbital hyperspectral imaging data from the Observatoire pour la Minéralogie, l'Eau, les Glaces et l'Activité (OMEGA) [5] onboard Mars Express and the Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) [6] onboard Mars Reconnaissance Orbiter (MRO) have revealed diverse and complex products of aqueous alteration, including hydrated sulfates, phyllosilicates, and hydrated silica. The discovery of these minerals has shed considerable light on Martian ancient aqueous history. Although the initial mineral identifications and analyses provided clues to their alteration environments, the mineral assemblages comprising the sediments and the relative abundances of the single minerals can further provide unique constraints to their formation environments. Mineral abundance estimates through spectral mixture analysis of orbital hyperspectral data have become necessary to further our understanding of the geologic history of Mars, although unmixing a reflectance spectrum into mineral abundance in an unambiguous way is difficult.

In this study, we perform spectral mixture analysis on CRISM data that have been atmospherically corrected for both gases and aerosols using radiative transfer modeling. Although mixing of reflectance spectra in the VNIR region has been shown to be non-

linear [7-10], conversion of reflectance data to single scattering albedo (SSA) allows for linear unmixing [11]. To do so, we atmospherically corrected CRISM I/F spectra using the Discrete Ordinate Radiative Transfer (DISORT) code by simultaneously modeling Mars atmospheric gases, aerosols, and surface scattering. SSAs were retrieved assuming that surface scattering can be modeled using the Hapke bidirectional scattering function [12]. Because single scattering albedos add linearly, a library of mineral SSAs (generated using mineral optical constants and assumed mineral grain sizes) were used for linear spectral unmixing of CRISM SSAs. Using this technique, we conducted a case study over Melas Chasma (Figure 1), where hydrated sulfates, jarosite and phyllosilicates have been all identified [13,14]. We then used the inferred mineral abundances to better constrain their extent, formation mechanisms, and the regional alteration environment.

Data Reduction Methodology: We use the Discrete Ordinate Radiative Transfer model (DISORT) to photometrically and atmospherically correct the CRISM data to retrieve single scattering albedos [15, 16]. The spectral end-member library of single scattering albedos used in this study is the one that cannot be directly measured. The single scattering albedo (SSA) is dependent on the optical constants (the real and imaginary indices of refraction n and k), which define a mineral's optical properties and grain sizes. To make the spectral library of the single scattering albedos, mineral optical constants were first obtained using the Shkuratov radiative transfer model [17, 19, 20] or the Hapke radiative transfer model [12, 19, 20]. To perform the spectral unmixing, the atmospherically corrected CRISM single scattering albedos were modeled using the non-negative least squares (NNLS) method [18] through the open source software package DaVinci, which is maintained by the Mars Space Flight Facility at Arizona State University (<http://davinci.asu.edu>) in partnership with other institutions. For each CRISM single scattering albedo spectrum, the model must reproduce the shape and depth of each of the absorption bands, the spectral continuum, and the absolute value of the reflectance. The script runs the model over all possible combinations of spectral end-member single scattering albedos and selected grain sizes, excluding unwanted end-members and grain sizes. Note that the grain size is not a free parameter in our model. This method has one advantage over the downhill simplex

minimization method because more control over the process of minimization is exerted by avoiding unrealistic grain sizes for certain phases which gives more reliable results. Spectra were modeled through several iterations to produce the best mathematical and visual fit by optimizing for the lowest RMS error between the retrieved and the modeled single scattering albedos, providing mineral abundances and grain sizes for each spectrum.

Results and Discussion: In the southern wall and nearby floor of Melas Chasma, a interbedded poly- and monohydrated sulfate unit (interbedded unit 1) in the ILDs was identified and interpreted to have formed either by cyclic evaporation and precipitation of the two hydrated sulfate phases from two episodic brines with different water chemistry, or through two precipitation-dehydration stages from a single complex Mg-Ca-Fe-SO₄-Cl brine [13]. Our spectral mixture analysis results show that polyhydrated sulfates within the interbedded unit 1 have much lower abundances (~13%) than the surrounding polyhydrated sulfates (21%) (Figure 2), which indicates that polyhydrated sulfates in the interbedded unit 1 might have been partially dehydrated into kieserite to form the interbedded strata and thus supports the two staged precipitation-dehydration formation hypothesis. Two jarosite-bearing units were also identified with one unit featured with a 2.265 μm absorption feature (unit 1) and the other unit (unit 2) featured with a deep 1.9 absorption feature in addition to a 2.265 μm feature. In the jarosite-bearing unit 1, the spectral unmixing results show that there is ~12% jarosite intermixed with significant amount of ferrihydrite with ~28% volume abundance whereas the jarosite-bearing unit 2 contains substantial schwertmannite (34%) in addition to jarosite and ferrihydrite. The jarosite and ferrihydrite assemblage in jarosite-bearing unit 1 could have coprecipitated during the evaporation of an acidic fluid where the originally precipitated schwertmannite has entirely transformed into other phases upon changing aqueous conditions. It is unclear if goethite is also present due to the possible spectral masking effects from ferrihydrite and schwertmannite [21].

Fe/Mg-smectites were also identified in southwest Melas Chasma to be interbedded with hydrated sulfates (interbedded unit 2) [14]. Our spectral unmixing results indicate that there are ~40% nontronite and ~20% hydrated sulfates in the interbedded strata. Together with the geochemical modeling results performed in Liu et al. [14], *in situ* coupled basalt weathering and evaporation may have initially produced similar amount of Fe/Mg smectites and polyhydrated sulfates, and the partial dehydration of polyhydrated sulfates into kieserite could have reduced the sulfate to clay

volume ratios to ~0.5. The consistency between geochemical modeling and spectral unmixing results and the lack of the evidence of the detrital origin of the clays indicate that Fe/Mg smectites as observed in southwest Melas Chasma are likely authigenic clays.

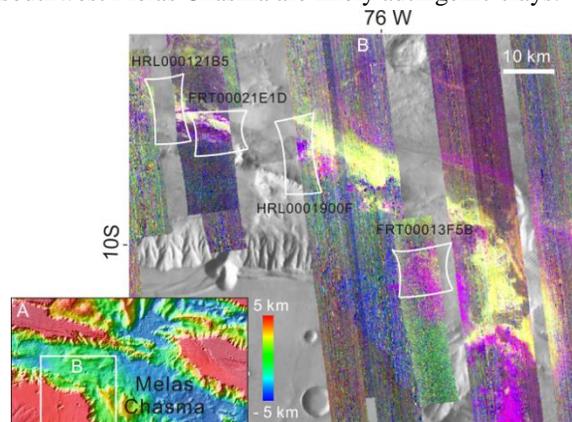


Figure 1. Southwest Melas Chasma. CRISM multiple parameter maps overlaid on THEMIS daytime mosaic. Red represents polyhydrated sulfates and yellow represents monohydrated sulfates. The inset for regional context is MOLA topography on a hill shaded map and southwest Melas Chasma is indicated by the white box.

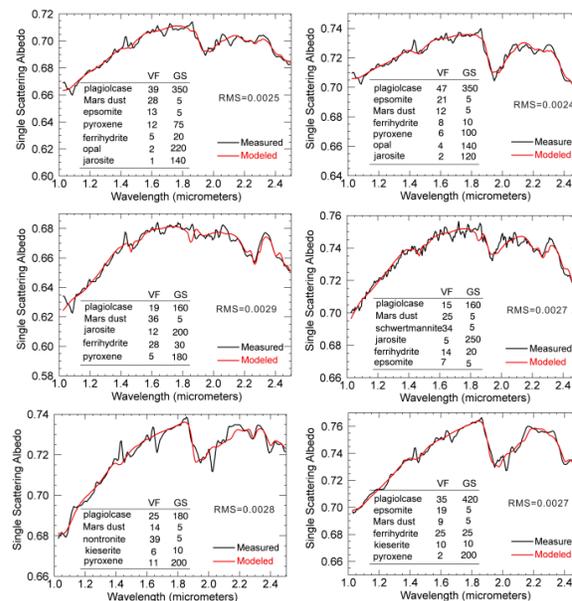


Figure 2. Derived mineral abundances (VF) and grain sizes (GS): (a) polyhydrated sulfate inside interbedded sulfate unit, (b) polyhydrated sulfate outside interbedded sulfate unit, (c) jarosite-bearing unit 1, (d) jarosite-bearing unit 2, (e) Fe-smectites in the interbedded clay and sulfate unit, (f) sulfates in the interbedded clay and sulfate unit.

References: [1] Keshava and Mustard, 2002; [2] Adams et al., 1986; [3] Roberts et al., 1993; [4] Somers et al., 2001. [5] Bibring et al., 2005; [6] Murchie et al., 2007; [7] Nash and Conel, 1974; [8] Singer, 1981; [9] Clark, 1983; [10] Johnson et al., 1992; [11] Hapke, 1981; [12] Hapke, 1993; [13] Liu et al., 2016a; [14] Liu et al., 2016b; [15] Stamnes et al., 1998; [16] Wolff et al., 2007; [17] Shkuratov et al., 1999; [18] Rogers and Aharonson, 2008; [19] Martone and Glotch, 2014; [20] Sklute et al., 2015; [21] Cull et al., 2014