Multivariate Spectral Analysis of CRISM Data to Characterize the Composition of Mawrth Vallis

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Introduction. Phyllosilicate deposits on Mars provide an opportunity to evaluate the aqueous activity as well as the possibility that habitable environments may have existed in the past. One of the prime locations for this type of study is Mawrth Vallis because of its abundant phyllosilicate outcrops and wealth of aqueous minerals [1]. Images taken with a high-resolution stereo camera (HRSC) allows us to see that the Mawrth Vallis is located within bright and dark regions, which formed during the Noachian period (4.1-3.7 Ga), a time when it was likely that water existed on Mars [1,2]. Additionally, [1] characterized the stratigraphy for the clay deposits within Mawrth Vallis using the Compact Reconnaissance Imaging Spectrometer for Mars (CRISM). These studies established the presence of various minerals such as nontronite, Fe²⁺ clays, sulfates, Al-phyllosilicate/opal, and allophane [1].

Thus far, analyses of this region have focused on the long wavelength (NIR, $\sim 1.0 - 4.0 \mu m$) CRISM data where overtones of phyllosilicates and sulfates are prominent. Inspired by [3,4], this study aims to incorporate additional spectral analysis techniques through the use of varimax-rotated, principal component analysis (VPCA) and forward stepwise linear regression on the visible/near-infrared spectral data obtained from CRISM in order to identify the minerals present in short wavelength (VNIR, $\sim 0.35 - 1.0 \ \mu m$) data that is dominated by oxides and Fe³⁺, Fe²⁺ minerals. The data reduction methods simplifies a multivariate data set by reducing it to a smaller number of independent linear combinations of the correlated input variables. If successful, this may allow a new opportunity to derive mineralogy from the short wavelength spectra.

Methods. The visible/near-infrared (VNIR) and nearinfrared (NIR) spectral data from CRISM were processed from the Planetary Data System (PDS) using CRISM Analysis Tools (CAT) through ENVI + IDL for the image 0000AA7D. Image corrections were performed using the pipeline of [5]. Nine regions of interest (ROI) were established in the IR data (Figure 1). To prepare the spectral data for VPCA, the average of the spectral reflectance values of adjacent bands were calculated, which decreased the spectral resolution, while increasing the signal to noise ratio. Then centerweighted derivatives were calculated from the spectral reflectance values of each sample to remove scattering effects [3,4]. The values were then processed through SPSS Statistics Software to undergo a varimax-rotated, principal component analysis to produce uncorrelated multivariate statistical results following the process of [6]. We input wavelengths of 0.39 to 1.05 microns. The

extraction of the VPCA was based on eigenvalues greater than one with a maximum of 25 iterations for convergence. This was followed by a final varimax-rotation, rotation step, which maximizes the squared loadings on as few of the input variables as posspible in each component.

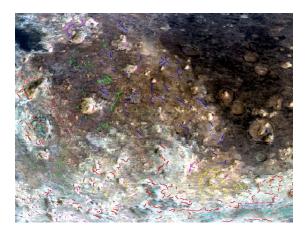


Figure 1: Nine ROIs were established in image 0000AA7D. The ROIs are as follows: Region 1 [1932 points, red], Region 2 [377 points, green], Region 3 [279 points, blue], Region 4 [261 points, yellow], Region 5 [378 points, cyan], Region 6 [425 points, magenta], Region 7 [255 points, maroon], Region 8 [297 points, sea green], Region 9 [147 points, purple].

To identify each component, a forward, stepwise multiple linear regression was performed through SPSS on the VPCA results to compare the extracted component spectra with standard derivative mineral spectra from the CRISM spectral library. This was done by comparing the z-score fit of the predictor standard minerals modeled by the multiple linear regression with the z-score of the extracted components. For this study, it is important to note that the absorption and reflectance processes in the visible part of the spectrum (400-700nm) are different from that in the NIR part of the spectrum (700-1000 nm). In the visible spectrum, absorption is dominated by electron transfer processes [6]. However, in the NIR, absorption is dur to the vibration of chemical bonds and their overtones and combinations. As a result, the correlation structure may be influenced differently across the wavelengths used in this study.

Results. Six components were identified from the VPCA (Figure 2) and their occurrence by ROI is represented by the varimax-rotated principal component

analysis (VPCA) score (Figure 3). Positive scores represent above average contribution for a given component in that ROI, while negative scores represent below average contributions. Values of zero represent average contributions.

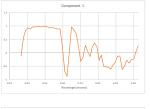


Figure 2: Example rotated component matrix values plotted for Component 1 extracted from the VPCA.

Figure 3: Example VPCA scores for Component 1 were plotted to determine the distribution of this particular score within each ROI. The colors correspond to those indicated for each ROI in Figure 1.

The mineral makeup of each of the components was identified by stepwise, forward multiple linear regression of each component against the predictor mineral standards. The following minerals were identified as present in the various components: palagonite, chlorite, pyroxene, nontronite, allophane, jarosite, and fayalite (Figure 4).

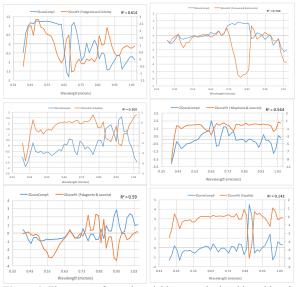


Figure 4: The z-score for each variable was calculated by taking the difference of a sample value and mean then dividing by the standard deviation. The z-scores for each component were plotted with the z-score fit values of the corresponding predictor minerals extracted from the forward stepwise linear regression. The R²values are indicative of how well the z-score of the component fits with the z-scores of the predictor standard minerals.

Discussion. The component scores represent the projection of standardized, partial correlation coefficients.

the component loadings onto the image data. To spatially understand the distribution of each component throughout the image 0000AA7D, the VPCA scores were analyzed with respect to ROIs. Component 1, which was interpreted to contain palagonite and chlorite, has relatively high VPCA scores of 1.59 and 1.30 in ROI1 and ROI6. The presence of palagonite and chlorite suggests that the deposits in this region were possibly volcanic and altered by aqueous activity in the past [7]. Component 2 was interpreted to contain pyroxene and nontronite and is principally found in ROI9 and ROI6. The presence of these minerals may be indicative of a basaltic source that may have chemically weathered into nontronite [8]. Components 3 and 6 both were interpreted to contain fayalite. The fayalite represented by Component 3 was found mostly in ROI2, which was the darkest region sampled in this study and has been interpreted to be possible lava flows [1,2]. Component 4 was interpreted to contain allophane and jarosite. This component was found mostly in ROI4. Both allophane and jarosite are hydrous minerals, which are strong indicators for the presence of water. The majority of these minerals were found adjacent to the palagonite deposits, further supporting that the deposits in ROI1 were altered by water. Finally, Component 5 was interpreted to contain palagonite and jarosite. The coexistence of these minerals indicate the presence of water as jarosite is a hydrous sulfate and palagonite is indicative of alteration by water. The spatial extent of Component 5 exists mostly in ROI7.

The lack of fit between the components and the identified mineral standards indictes that there are likely additional minerals present in the samples that have yet to be identified. Despite this, these results compare reasonably well with previous studies in that iron-rich phylosilicates, such as nontronite, have been detected in the local regions of 0000AA7D [1]. Additionally, this study supports the evidence for palagonitic minerals as evidence of the various degrees of weathering on the surficial basaltic rocks [7].

Conclusions. We show that spectral signatures of palagonite, pyroxene, chlorite, nontronite, allophane, jarosite, and fayalite can be detected in VNIR spectra using VPCA and forward stepwise linear regression analysis. This provides a new method to derive mineralogy from the short wavelength CRISM data, which currently are not utilized as extensively as the NIR data. The minerals identified via this process are dominated by aqueous minerals and are consistent with those found in previous studies of this region in the NIR data. References. [1] Bishop, J. L. et al. (2013) Plan. Space Sci. 86, 130. [2] Loizeau, D. et al. (2007), JGR 112.[3] Ortiz, J. et al. (2017) Front. in Marine Sci.4, 296. [4] Ortiz, J. et al. (2013) Int. J. Remote Sens. 34. [5] Murchie, S. et al. (2007), JGR 112 [6] Yurco, L. N., et al.. (2010) Polar Res., 29, 176. [7] Morris et al. (2001) JGR, 106, 5057. [8] Gainey, S.R. et al. (2014) Geo. et Cos. Acta 126, 192-211.