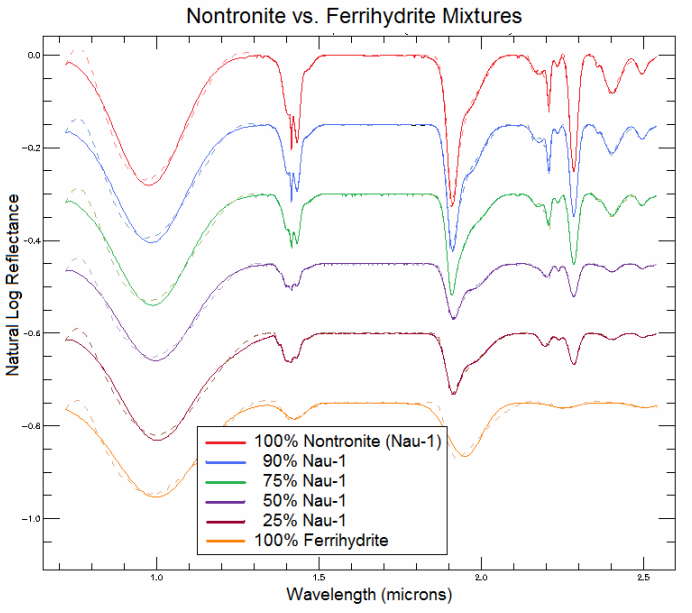
DETERMINING THE COMPOSITION OF PHYLLOSILICATES USING AUTOMATED GAUSSIAN MODELING OF SPECTRAL FEATURES. Heather D. Makarewicz[1,2,4], Mario Parente[2,3], and Janice L. Bishop[2,4], [1]University of Kansas, Lawrence, KS, [2]SETI Institute, Mountain View, CA, [3]Stanford University, Stanford, CA, [4]NASA ARC, Moffett Field, CA.

Introduction: Phyllosilicates have been detected in several regions on Mars using the hyperspectral visible/near-infrared (VNIR) imagers OMEGA [1] and CRISM [2]. Lab studies of phyllosilicate mixtures have been found to replicate well the character of the phyllosilicate-bearing spectra collected using CRISM [3,4]. Here we extend these studies using Modified Gaussian Model (MGM) analysis in order to determine the composition of specific endmembers in the spectra.

This is achieved through a newly developed automated method. This new method builds on the MGM technique [5,6] that has been successfully applied to hyperspectral analyses of Mars [7,8]. However, these models require user-selected initial parameters. Initial efforts in automating this modeling process for CRISM hyperspectral images have been successful, but are limited to the study of pyroxene bands at 2 µm [9]. This technique has been extended to model spectral features using Gaussians from 0.5-2.6 µm. An automatic parameter initialization step based on the features of the spectrum being modeled is used in order to further automate MGM modeling. Two phyllosilicate mixtures are analyzed using the automated MGM for this study. These are laboratory mixtures of kaolinite with montmorillonite and nontronite with ferrihydrite. The objective of this study is to extend the work of Sunshine, et. al. in determining composition of minerals using the MGM method [6,10].

Methods: A method for automatic parameter initialization for the MGM was developed. First, the continuum is modeled and removed using a linear spline interpolation over the set of points found from computing a convex hull over the natural logarithm of the spectrum. Next, the initial Gaussians for the MGM are determined. This is accomplished by computing the 1st and 2nd derivatives of the spectrum and locating local extrema and inflection points. Each derivative is preceeded by a filter to minimize the amplification of noise [11]. Some inflection points are retained as band centers for starting Gaussians. These inflection points and the minima form the set of initial band centers. Next, the band depths are calculated by taking the difference between the global maximum and the spectrum value at each band center. The full width at half maximum is approximated as half the width at the base of the Gaussian, which is assumed to be the distance between the two neighboring band centers. Finally, the band strength is found using an approximation of the area of each Gaussian. These estimates together with the band centers give the initial Gaussian parameters. The initial Gaussians are then optimized over the continuum-removed spectrum using the total inversion least squares method described by Tarantola and



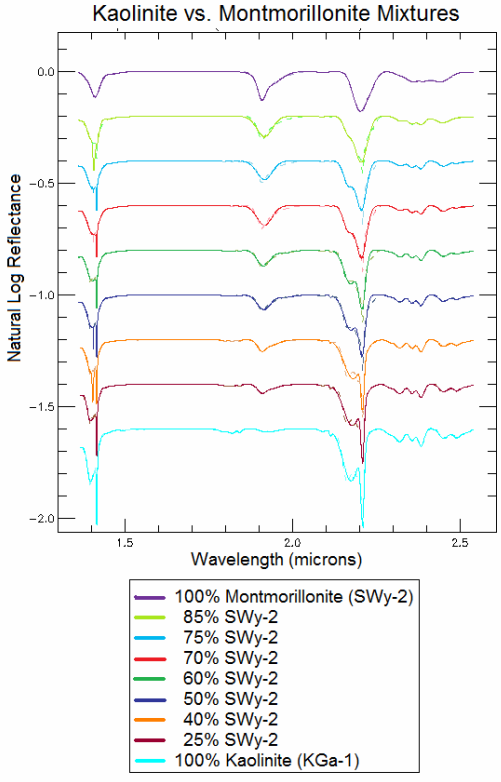


Fig 1,2: Continuum Removed Mixture Spectra and Fits

Valette [12]. This method differs from the MGM since the continuum is modeled and removed first, and the Gaussians are then optimized over a continuum removed spectrum.

Samples and spectra: Reflectance spectra of the mixtures were acquired at RELAB/Brown University, as in previous studies [e.g. 13]. Continuum-removed versions of these spectra are shown in Figures 1 and 2. The kaolinite plus montmorillonite mixtures were prepared by wt.% [14] as were the nontronite plus ferrihydrite mixtures [4]. All the mixture spectra were modeled using the automated MGM method.

Results: *Kaolinite-Montmorillonite.* Kaolinite spectra have doublet features that are modeled well at 1.39 and 1.41 µm and at 2.17 and 2.21 µm. Montmorillonite spectra have three major asymmetric absorptions at 1.41, 1.91, and 2.21 µm. For mixture spectra, several relationships between band depths have been found which can predict composition. Figure 3 shows the linear relationships found comparing band depths. No significant relationships were found for band centers or widths.

Nontronite-Ferrihydrite. Nontronite spectra have composite features that are modeled well at 1.40/1.41/1.42 and 1.91/1.95 µm and a band at 2.28 µm, while ferrihydrite spectra have features at 1.43 and 1.95 µm. Figure 4 shows the linear relationships found comparing band depths. No significant relationships were found for band centers or widths.

Summary: An algorithm was created which automatically generates starting parameters for the modified Gaussian model. This method was utilized to analyze composition of kaolinite-montmorillonite and nontronite-ferrihydrite mixtures. Several relationships were found that relate relative band depths with endmember composition. Ongoing work involves extending this technique to other mixtures, testing on known phyllisilicate mixtures, and remote data.

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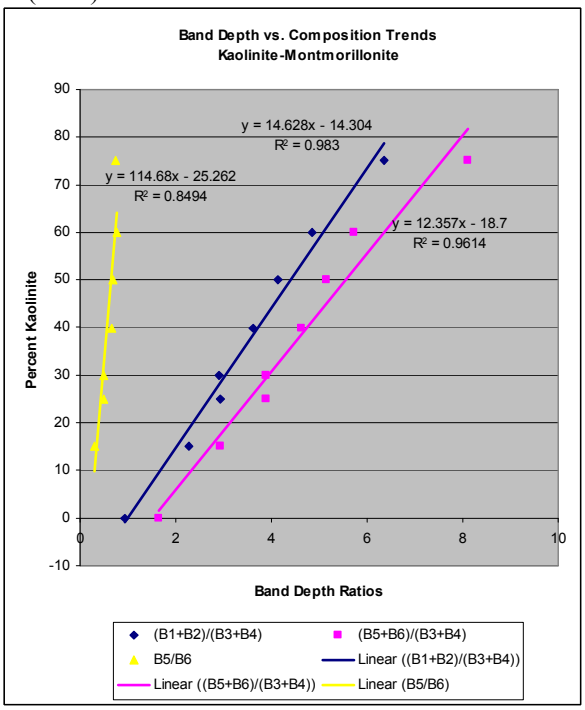

Fig 3: Compositional Trends by Band Depth Ratios B1, B2, B3, B4, B5, B6 are the depths at the 1.39, 1.41, 1.91, 1.93, 2.17, 2.21 µm features, respectively.

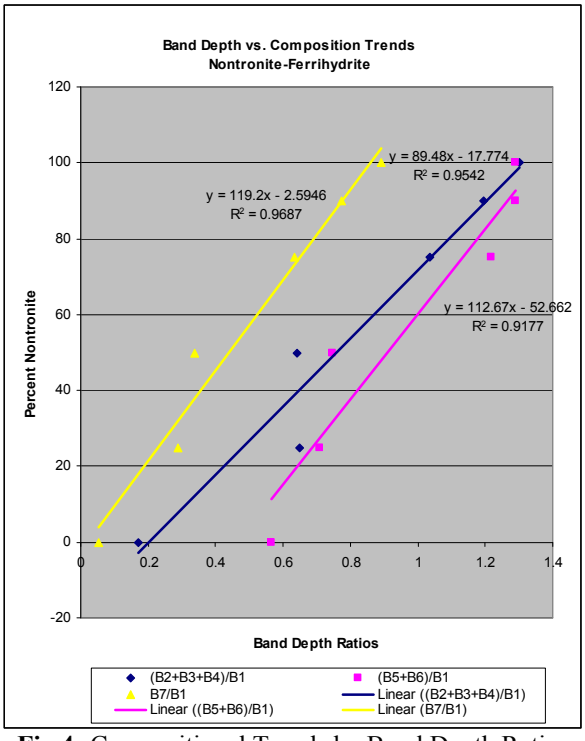

Fig 4: Compositional Trends by Band Depth Ratios B1, B2, B3, B4, B5, B6, B7 are the depths at the 0.98, 1.40, 1.41, 1.43, 1.91, 1.95, 2.28 µm features, respectively.