APPLICATION OF DEEP LEARNING AND SPECTRAL DECONVOLUTION FOR ESTIMATING MINERAL ABUNDANCES OF ZEOLITE, MG-SULFATE AND MONTMORILLONITE MIXTURES AND ITS IMPLICATIONS FOR MARS. G. R. L. Kodikara, and L. J. McHenry, Dept. of Geosciences, University of Wisconsin- Milwaukee, Milwaukee, WI 53211, gayantha@uwm.edu, lmchenry@uwm.edu.

Introduction: Based on the spectral characteristics captured by the orbital spectral sensors, hydrous minerals, such as smectites, kaolinite, sulfates, carbonates, zeolites, opaline silica, chlorites, serpentine, prehnite and epidote have been identified on the surface of Mars (e.g. [1,2]). [1] identified the Na-zeolite analcime in the Nili Fossae region on Mars using Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) data. Analcime is the only zeolite group mineral identified on Mars based on its distinctive broad absorption band centered at ~ 2.5 μm and a weaker absorption at ~ 1.8 μm [1,2]. These studies show the difficulties associated with identifying other zeolite minerals using orbital spectral data. Identification of other zeolite species is complicated by the lack of diagnostic absorption bands in the visible-shortwave infrared (VIS-SWIR) region [2], spectral similarity with Mg-polyhydrated sulfates [1], and residual atmospheric effects at wavelengths longer than 2.5 μm [4]. [2] noted that the only ways to discriminate polyhydrated sulfates from zeolites are to use the position of the 2.3 - 2.4 μm shoulder and the shape of the 1.9 μm absorption. However, in most studies, non-analcime and polyhydrated sulfates are commonly categorized as an unidentified hydrous phase (e. g. [5]), or as zeolite and sulfate group (e. g. [2]).

In this study, a technique for estimating clinoptilolite (a zeolite mineral), montmorillonite, and epsomite (a Mg-polyhydrated mineral) mineral abundances from a reflectance spectrum of mineral mixtures using spectral deconvolution and a deep neural network is presented.

Methods: Sixty-six ternary mineral mixtures were physically prepared with < 150 μm grain sizes with different weight percentages of clinoptilolite, montmorillonite, and epsomite (Fig. 1). A combination of normal and skewed Gaussian curves was fitted to the absorption bands at 1.4 μm, 1.9 μm, and 2.2 μm of the acquired reflectance spectra of these mineral mixtures. Six Gaussian curve parameters with maximum absorption band depth ~ 1.9 μm, and wavelength at the maximum band depth, were used (along with mineral abundances) to train multilayer perceptron deep neural network (MLP-DDN) models. Forty-eight models with different DNN architectures and different hyperparameters were trained and the results were validated to find the best models. Winning models were tested with twenty-five samples including fourteen library spectra from RELAB and USGS spectral databases, a spectrum from a different sample, five varying amounts of noise-added spectra simulating CRISM (Compact Reconnaissance Imaging Spectrometer for Mars) orbital spectral data, and five mixed spectra derived from linear mixtures of laboratory minerals.

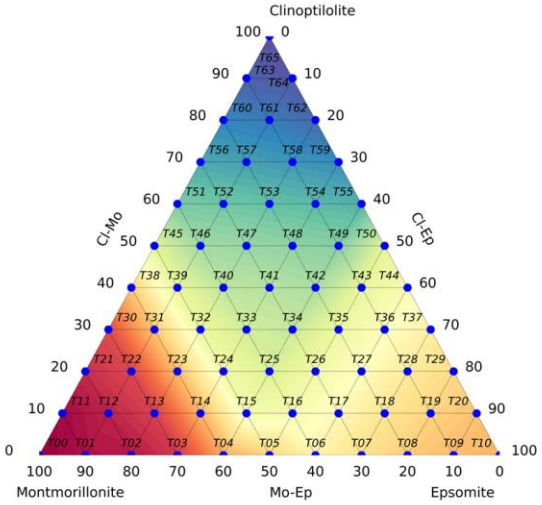

Figure 1. Schematic ternary diagram for mixtures of clinoptilolite, montmorillonite and epsomite. Blue points show the sample points of physical mineral mixtures prepared to collect reflectance spectra. The sample ID for each mixture is shown near the sample point.

The entire study was conducted using several python modules (numpy, math, lmfit, matplotlib, and pytorch) implemented in Rstudio IDE (integrated development environment) (https://www.rstudio.com). An open-source machine learning framework pytorch (https://pytorch.org/) was used to build deep learning models.

Results and discussion: The calculated maximum band depth of 1.9 μm absorption feature (F2BD_MAX), is graphically shown in Figure 2, as an example. It shows that the maximum band depth of the 1.9 μm absorption feature (F2) increases towards epsomite from both clinoptilolite (mainly) and montmorillonite.

From the 48 MLP-DNN models, two hidden layer architecture (with six units in each hidden layer) with ADAM optimization and Sigmoid activation function was selected as the best model based on its lowest root mean square error (RMS) yield with the validation of

test data. The selected DNN model was able to predict mineral mixture composition with higher accuracies; three of five montmorillonite and four of the five epsomite library spectra with more than 90 % of accuracy. However, clinoptilolite samples show less than 50 % accuracy and were always predicted as mixture of clinoptilolite and epsomite (Figure 3).

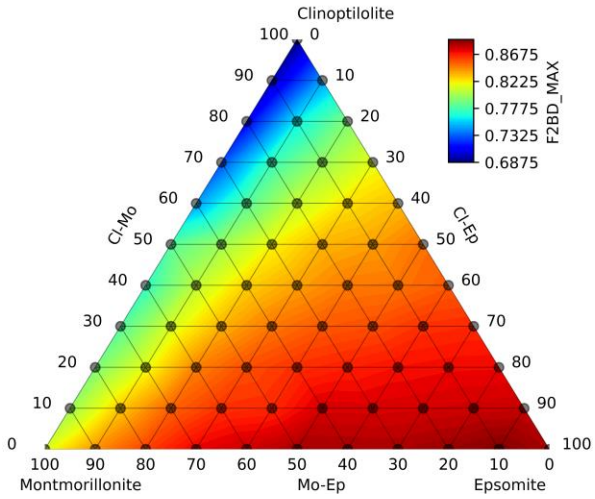

Figure 2. Ternary plots showing the maximum band depth of 1.9 μm absorption feature (F2BD_MAX).

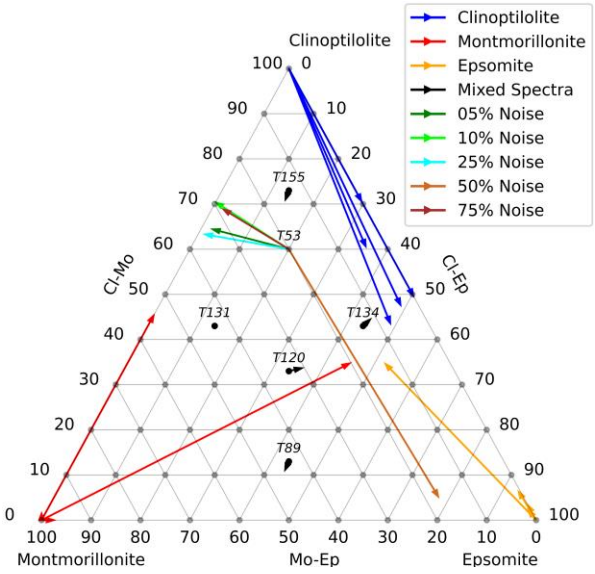

Figure 3. Ternary plot showing the original composition of the mineral/mineral mixture with their predicted compositions. Arrowheads show the predicted composition of each mineral mixture.

The study demonstrates the difficulties of identifying non-analcime zeolites (e.g. clinoptilolite) from Mg-polyhydrated minerals, as discussed by authors who have mapped hydrous minerals on Mars using hyperspectral image data. Random artifacts introduced by noise sometime leads to predictions of completely different and incorrect mineral abundances.

Conclusion: We have examined the efficacy of a combination of spectral deconvolution and deep neural network techniques to estimate mineral abundances of zeolite, Mg-sulfate and montmorillonite mixtures using their reflectance spectra. Key findings are as follows, 1) The presence of at least ~ 10% of montmorillonite in a clinoptilolite-montmorillonite mixture can entirely mask the presence of the clinoptilolite in SWIR spectral data. 2) In the sample contain higher than ~ 20 % of montmorillonite in an epsomite-montmorillonite mixture, it will mask the presence of the epsomite in SWIR spectral data. 3) The results show the difficulties of identifying clinoptilolite from epsomite even if the spectra were acquired under laboratory conditions. 4) The absorption bands at 1.4 μm, 1.9 μm, and 2.2 μm were able to mathematically deconvolve by two normal Gaussian curves, a normal Gaussian curve with a skewed Gaussian curve, and a normal Gaussian curve, respectively. 5) Selection of the correct input features, architecture of DNN, and hyperparameters help to predict the mineral abundances with higher accuracies. 6) Care must be taken when estimating mineral abundance from a new dataset, even from a well-trained DNN. The new dataset must have similar characteristics to the training dataset to achieve the best results. Normalizing the spectral parameters before feeding it to the DNN might be a good approach, if working with a wide variety of datasets. 7) It will be important to incorporate the contribution from albedo, particle size, water content, and cation substitution in future models.

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References: [1] Ehlmann et al. (2009) *JGR* 114. [2] Carter et al. (2013) *JGR: Planets*. 118. 831-858. [3] Cloutis et al. (2002) *JGR 107*. [4] Murchie et al. (2007) *JGR* 112. [5] Sun and Milliken (2015) *JGR* 120. 2293-2332.