PRINCIPLE COMPONENT ANALYSIS APPLIED TO REFLECTANCE SPECTRA OF MINERALS SUBJECTED TO ENVIRONMENT SIMILAR TO MARTIAN SURFACE. Joseph S. Makarewicz and Heather D. Makarewicz, Olivet Nazarene University, Bourbonnais, IL.

Introduction: Reflectance spectra from the OMEGA and CRISM visible/near-infared (VNIR) imagers continue to be analyzed. The classification process is complicated because the spectral features are affected by composition as well as environmental conditions. To study how spectral features are influenced by environmental conditions, laboratory spectra are collected in enviromnetal chambers emulating Martian surface conditions. In this study, we are applying principle component analysis (PCA) to a spectral suite collected in a Mars environment chamber at the Centre for Terrestrial and Planetary Exploration (C-TAPE) at the University of Winnipeg [1].

PCA applied Reflectance Spectra: PCA has been previously applied to mineral mixture datasets. It was applied to a pyroxene mixture dataset and was used to predict percent composition and grain size [2]. It was applied to two phyllosilicate-containing mixture datasets to understand how percent composition affects spectral features [3]. Percent composition was predicted for tertiary and quaternary mixture datasets containing silicates [4]. It was also shown that PCA can be used to virtually mix endmembers [5,6]. This study will show that PCA can also be applied to datasets where environmental conditions are varied.

Methods: *Samples and Spectra.* The Mars Box Run 1 ASD dataset was selected for this study. The dataset contains Calcite, Clinochlore, Gypsum, Hexahydrite, Jarosite, Nontronite, and Serpentine. The minerals were initially subjected to 5 Torr of dry CO_2 for 24 days followed by 8-20 milliTorr of dry CO_2 for an additional 25 days. Starting on Day 15, the samples were exposed to UV light from a deuterium lamp. The spectra were measured intermittently over the 49 day period. This dataset was collected for another study and reposed in the PSF spectral database [1].

Pre-processing. Aside from isolating individual spectra from the excel file, no pre-processing was required. The spectra span 0.35 to 2.5 µm wavelengths with a resolution of 1 µm. They were not cropped or resampled. The data was also not normalized. The Nontronite spectra are shown in Fig. 1.

PCA procedure. PCA was performed on each mineral individually using singular value decomposition (SVD). Before performing PCA, the mean spectrum for the mineral set was subtracted from each spectrum. The mean spectrum along with the most significant principle component vector for the Nontronite spectra is shown in Fig. 2. PCA also produced 16 principle component values corresponding to each day shown in Fig. 1. Each spectrum can be approximated as the mean spectrum plus the first principle component vector multiplied by the first principle component value. In Fig. 3, the principle component values for Nontronite are plotted against time. The first principle component value was related to the CO_2 pressure.

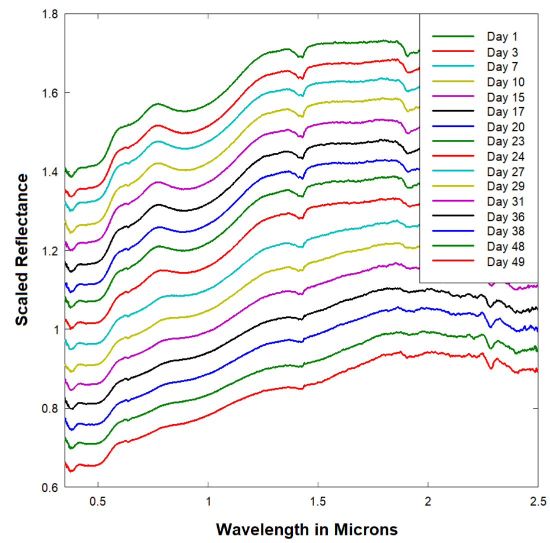

Fig. 1: PSF Mars Box Run 1 ASD Nontronite dataset with offsets.

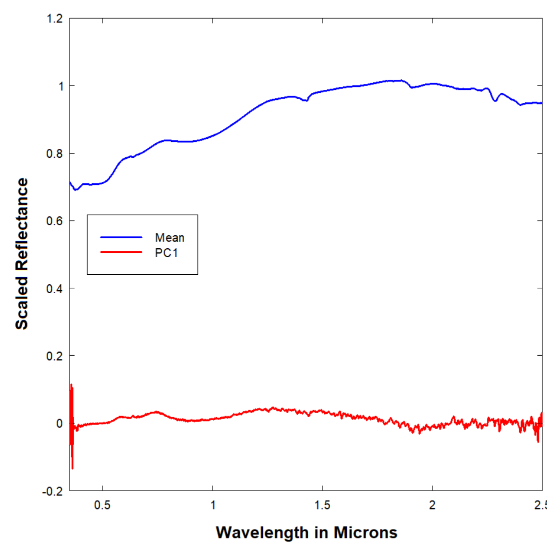

Fig. 2: Nontronite mean spectrum and first principle component vector generated by PCA.

Results: The methods were applied to each of the minerals. For some of the minerals, the first principle component was related to an enviromnetal condition. Table 1 shows which environmental condition was related to the first principle component for each of the minerals.

Mineral	PC1 Values
Calcite (<45µm)	-
Calcite (90-180µm)	-
Clinochlore	8-20 milliTorr CO_2 Pressure
Gypsum	8-20 milliTorr CO_2 Pressure
Hexahydrite	UV Light
Jarosite	-
Nontronite	8-20 milliTorr CO_2 Pressure
Serpentine	UV Light

Table 1: Environmental condition related to the first principle component.

For both Calcite samples, the PC1 vector has features in the 0.35 to 0.7 µm wavelength range. However, the PC1 values appear to be random and not related to the environmental conditions.

For the Clinochlore sample, the PC1 vector has features in the 0.35 to 0.5 µm wavelength range. After the low pressure CO_2 is turned on at Day 25, there is a slight increase n PC1 values.

For the Gypsum sample, the PC1 vector has features in the 1.4 to 2.4 µm wavelength range. After the low pressure CO_2 is turned on at Day 25, there is a distinct exponential increase in PC1 values.

For the Hexahydrite sample, the PC1 vector has features in the 1.4 to 2.4 µm wavelength range. After the UV light is turned on at Day 15, there is an increase in PC1 values.

For the Jarosite sample, the PC1 vector has no easily obsevable features. The PC1 values also appear to be unrelated to the environmental conditions.

For the Nontronite sample, the PC1 vector has notable features in the 0.5 to 0.9 µm wavelength range as seen in Fig. 2. After the low pressure CO_2 is turned on at Day 25, there is a distinct exponential increase in PC1 values, which can be seen in Fig. 3.

For the Serpentine sample, the PC1 vector has features in the 0.35 to 0.7 µm wavelength range. After the UV light is turned on at Day 15, there is an increase in PC1 values.

Discussion: For most of the minerals, PC1 accounts for more than 80% of the variation in the spectra. PC2 accounts for most of the remaining variation but the PC2 values appear to be unrelated to the environmental conditions.

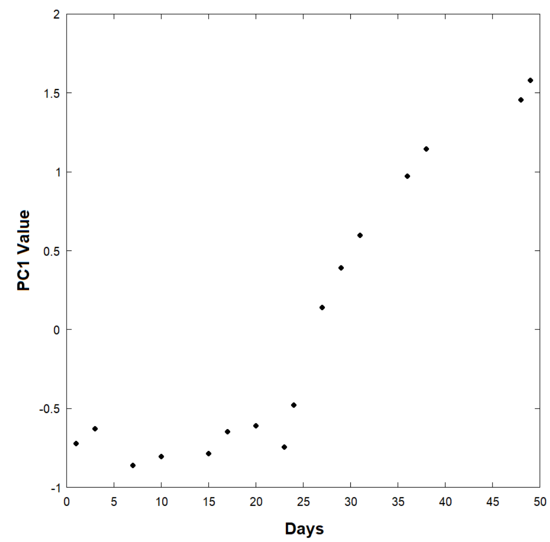

Fig. 3: A scatter plot relating the Nontronite first principle component value to time. At Day 25, the sample was subjected to 8-20 milliTorr of CO_2.

The spectra of the Jarosite and two Calcite samples all visually look similar. It is not surprising that PCA provided no additional information. This would imply Jarosite and Calcite spectra are unaffected in the 0.35 to 2.5 µm by CO_2 pressure and UV light.

This spectra for the Nontronite and Gypsum samples have drastic changes over the 49 day experiment. The PC1 values have very distinct exponential curves, showing that the spectra changes are quantifiable and predictable. Further research needs to be conducted to determine if the changes are permanent and why they are occurring.

Future Work: Only the Mars Box Run 1 ASD dataset was analyzed. Runs 2 - 6 could also be analyzed.

Summary: PCA is applied to a VNIR spectra dataset in which the samples were exposed to UV light and CO_2 at several pressures. The samples included Calcite, Clinochlore, Gypsum, Hexahydrite, Jarosite, Nontronite and Serpentine.

References: [1] Cloutis E. A. et al. (2008) Icarus, 195(1), 140-168. [2] J.S. Makarewicz and H.D. Makarewicz (2013) *IEEE Whispers* doi: 10.1109/WHISPERS.2013.8080604. [3] J.S. Makarewicz, H.D. Makarewicz, and J.L. Bishop (2018) LPSC, Abstract #1378, Poster #503. [4] D.J. Burnett and J.S. Makarewicz (2018) AGU Fall Meeting, Abstract #P41D-3767. [5] J.S. Makarewicz and H.D. Makarewicz (2018) AGU Fall Meeting, Abstract #IN11E-0665. [6] J.S. Makarewicz and H.D. Makarewicz (2019) LPSC, Abstract #2400, Poster #720.