EVALUATING CM CHONDRITE COMPOSITIONS USING MIR SPECTRA OF MINERAL MIXTURES AND MULTIVARIATE ANALYSIS. L. B. Breitenfeld[1], A. D. Rogers[1], and T. D. Glotch[1], [1]Dept. of Geosciences, Stony Brook University, Stony Brook, NY, laura.breitenfeld@stonybrook.edu.

Introduction: Estimating modal mineralogy for meteorites and asteroids is important for understanding compositional diversity and small body evolution in the early solar system. Meteorite composition can constrain the degree of aqueous alteration and/or thermal metamorphism experienced by the asteroid parent body. Mid-infrared (MIR) spectroscopy is a common telescopic, spacecraft, and laboratory tool used to determine mineral composition. Although mineral identification is possible through MIR spectroscopy, fine-particulates in the MIR do not mix linearly [1], making quantification difficult for some materials.

Multivariate analysis removes the assumption of linear mixing across wavelengths and is therefore useful for spectroscopic techniques in which non-linear mixing occurs. It has been utilized as an effective tool for evaluating compositional abundances using several types of spectroscopy [2–4]. This technique requires preparation of a training set covering the relevant compositions and particle sizes. We are constructing a fine-particulate (<50 µm) albedo-constrained library and training set for multivariate analysis. Here we present progress on the development of this training set of analog mixtures, some initial assessments of expected model accuracy, and plans for future work.

Sample Preparation: The mineral species utilized in this work are terrestrial samples commonly present within CM chondrites [5, 6]. These minerals include antigorite, cronstedtite, magnetite, pyrrhotite, olivine (Fo_{40}, Fo_{80}, Fo_{90}), calcite, dolomite, ferrihydrite, gypsum, and enstatite. Natural samples were hand-picked and in some cases were centrifuged, acid-washed, or magnetically separated to remove unwanted contaminants. Each was hand crushed or milled to create fine-particulate samples (<50 µm).

Currently, 54 mixtures have been analyzed. These samples include simple mixtures (35 binary and 4 ternary) and 15 analog CM chondrites mixtures. All samples (including end-members) were darkened using 11 vol% nanophase carbon powder to constrain the albedo to more closely match carbonaceous chondrites, as visible albedo can have a strong effect on MIR spectral properties.

Instrumentation: MIR spectra were acquired in a simulated asteroid environment (SAE) using the Planetary and Asteroid Regolith Spectroscopy Environmental Chamber (PARSEC), a custom-built planetary environmental spectroscopy chamber at Stony Brook. PARSEC is coupled to a Nicolet 6700 FTIR spectrometer for emissivity measurements. For SAE measurements, the chamber was pumped to ~10^{-4} mbar and cooled to <125 °C. Samples were heated to 80 °C.

Machine Learning Models: Using end-members and mixtures, partial least squares machine learning models were constructed, as in [7, 8]. The accuracy of each model was evaluated using the parameter leave-one-out cross-validated root mean square error (LOO RMSE-CV). This metric is calculated by removing one sample at a time, using a regression model based on the other n–1 samples to predict the nth sample. LOO RMSE-CV gives the best estimate of how the model will perform on unseen data. LOO RMSE-CV range from 4.4–17.0 vol%. Model accuracies depend on the parameters utilized (e.g., wavenumber range) and prediction mineral in question. As spectra are added to the multivariate models, the errors will change.

Murchison Unmixing: A MIR SAE spectrum was collected of the CM chondrite Murchison (<45 microns) under identical conditions to the training set. Using the PLS models, modal mineralogy predictions were made. Several species were accurately predicted within 5 vol% compared to literature values [5, 6]. These species include antigorite, Fo_{40}, Fo_{80}, enstatite, calcite and gypsum. Dolomite and ferrihydrite were not included in other worker's estimates [5, 6] and our prediction values of <2vol% for each species is consistent. Other minerals like Fo_{90}, pyrrhotite, magnetite and cronstedtite were either over or underestimated in our model by >5 volume%. With the addition of more samples within the model, the model error is expected to reduce while prediction accuracy improves.

Implications and Ongoing Work: The machine learning spectral unmixing models developed here may be applicable to telescopic observations of asteroids, spectral data from missions like OSIRIS-REx and non-destructive laboratory investigations of meteorites.

This training set will be expanded by creating more analog mixtures and integrating synthetic coarse-particulate spectra to predict compositions over a range of particle sizes. Saponite will be added to the model as an end-member to expand the applicability of this work to CI chondrite unmixing. VNIR spectra will be collected for all samples to create an equivalent model. Lastly, PLS models will be applied to additional chondrites to test model accuracy on unseen data.

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