EVALUATING BENNU'S SURFACE COMPOSITIONS USING MIR SPECTRA OF FINE-PARTICULATE, ALBEDO-CONSTRAINED MINERAL MIXTURES AND MULTIVARIATE ANALYSIS.

L. B. Breitenfeld[1], A. D. Rogers[1] , T. D. Glotch[1] , V. E. Hamilton[2] , P. R. Christensen[3] , and D. S. Lauretta[4], [1]Dept. of Geosciences, Stony Brook University, Stony Brook, NY, laura.breitenfeld@stonybrook.edu, [2]Dept. of Space Science, Southwest Research Institute, Boulder, CO, [3]School of Earth and Space Exploration, Arizona State University, Tempe, AZ, [4]Lunar and Planetary Laboratory, University of Arizona, Tucson, AZ.

Introduction: Detailed assessment of the asteroid Bennu's mineralogy and compositional variability is broadly applicable to the study of carbonaceous near-Earth asteroids and primitive material within our solar system. Among the chondrites, the spectral properties of Bennu are most analogous to those of CI or CM (carbonaceous) chondrites [1–4]. The OSIRIS-REx spacecraft hosts the OSIRIS-REx Thermal Emission Spectrometer (OTES) instrument [5] that observes Bennu in the mid-infrared (MIR) and can be utilized for further refining Bennu's mineralogy [e.g. 4].

Using linear mixing models [6,7], mineral abundance estimates from fine-particulate surfaces (<60 microns) generally have reduced accuracy compared to coarse-particulate surfaces; however, improvements may be possible using multivariate analysis. This is because this alternative approach removes the assumption of linear mixing across all wavelengths. Multivariate analysis requires preparation of a training set covering the relevant compositions and particle sizes. This technique has been proven to be an effective tool for evaluating compositional abundances using several types of spectroscopy [8–10]. To prepare for any possible detections of fine-particulate materials in OTES data, we are constructing a fine-particulate (<50 microns) 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 CI and CM chondrites [11–13]. These minerals include antigorite, cronstedtite, magnetite, pyrrhotite, olivine (Fo_{40}, Fo_{80}, Fo_{95}), calcite, dolomite, ferrihydrite, gypsum, and enstatite. In addition to these end-members, saponite will be added to this model in the upcoming months. Suitable samples were obtained from several museum collections and dealers or synthesized at Stony Brook. Natural samples were hand-picked for purity 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 microns).

Mixtures: Currently, 54 mixtures have been analyzed (**Figure 1**). Saponite-bearing mixtures are not yet available. This precludes immediate application to OTES spectra at this time.

The suite of 12 minerals common in CI and CM chondrites [11–13] was utilized as end-members within the multivariate analysis models. All samples were darkened using 11 vol% nanophase carbon powder to constrain the albedo of the samples to more closely match Bennu's visible albedo.

Using these samples, analog CI and CM meteorite mixtures were made using modal abundances that encompass literature values [4,11,12]. Binary and ternary mineral mixtures were also made. Using binary and ternary mixtures in this project is helpful for:

1. Isolating complex mixing effects for the multivariate model.
2. Ensuring every mineral in the model has several data points between 0 and 100 vol%.

This second point is important, because although narrower model ranges can allow for precise predictions, a restricted model could bias prediction results and would be unable to detect true compositional outliers accurately (higher or lower mineral abundance than in typical CI or CM chondrites).

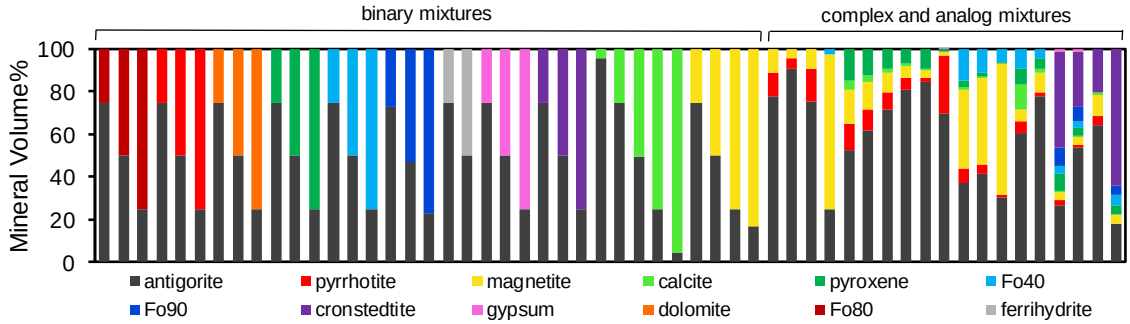

Figure 1. Mineral abundances of binary and CM analog mixtures complete thus far in volume%. These abundances have been normalized to remove the 11 volume% of carbon powder that is present in each mixture.

Instrumentation: MIR spectra were acquired in a simulated asteroid environment (SAE). For these measurements, we utilized the Planetary and Asteroid Regolith Spectroscopy Environmental Chamber (PARSEC), a custom-built planetary environmental spectroscopy chamber at Stony Brook University. PARSEC is coupled to a Nicolet 6700 FTIR spectrometer for emissivity measurements. Before SAE measurements, the chamber was pumped to ~10^{-4} mbar over several hours and subsequently cooled to <125 °C. Blackbody measurements were acquired at 70 and 100 °C while samples were heated to 80 °C.

Laboratory Spectral Trends: For the binary mixtures, feature strength is correlated with the relative volume percentage of the given component. However, non-linear mixing effects are present within this data set as expected for MIR emission spectra of fines [6]. Individual mineral features are nearly always obscured in mixtures with more than two components.

Spectra of mixtures analyzed thus far that have mineral abundances similar to CM chondrites do not perfectly match the OTES data collected in preliminary survey [4] (**Figure 2**). This is expected because this whole-disk spectrum is dominated by coarse particulates clearly present on Bennu. These analog spectra possess a feature with a similar shape to the 440 cm^{-1} Bennu absorption [e.g. 4] but it is offset to higher wavenumbers. The 555 cm^{-1} magnetite feature observed on Bennu is detectable in the laboratory spectra at volume percentages as low as 3.4%. The Christiansen Feature (CF) wavenumber positions vary yet all mixtures possess a "roll-off" diagnostic of fine particulates shortward of the CFs.

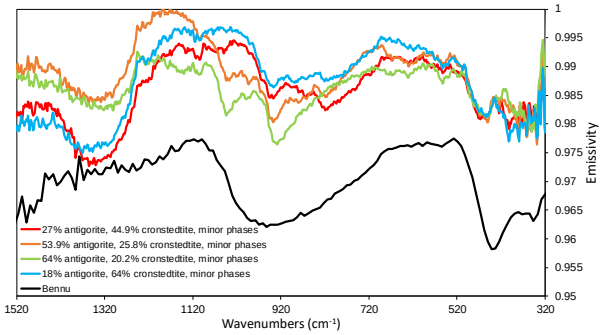

Figure 2. SAE MIR spectra of CM analog mixtures in vol% and OTES global average spectrum of Bennu [4]. Four mixtures correspond with the samples on the right of Figure 1 and are shown at laboratory spectral resolution. The listed mineral abundances normalize out the carbon powder present.

Multivariate Analysis: MIR spectra of the 12 darkened samples act as end-members within the multivariate models. In addition to these data, spectra of mixtures were evaluated with partial least squares machine learning models, as in [14,15].

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 since this error is calculated from predictions that do not rely on itself.

LOO RMSE-CV range from 4.5–17.0 vol%. Model accuracies depend on the parameters utilized (e.g., wavenumber range) and prediction mineral in question. The creation of these multivariate models is ongoing. As spectra are added to the multivariate models, the errors will change.

Ongoing Work: This training set, spectral data set, and multivariate model will be expanded in three ways.

1. Adding the end-member sample, binary mixtures, and analog mixtures using saponite.
2. Creating additional CI and CM analog mixtures.
3. Integrating synthetic coarse-particulate spectra to predict compositions over a range of particle sizes.

The resulting multivariate model will be applied to spectra of fine-particulate CI and CM meteorite samples once the training set is completed. Testing models on "unseen" data (spectra not part of the training set) is an important step to validate the accuracy of the model and for choosing the most appropriate model.

In addition to predicting the bulk mineralogy of Bennu, these models will be applied to regions of Bennu with surfaces showing evidence for a greater proportion of fine particles, such as the areas previously considered as possible sampling sites, in addition to the selected primary sampling site, known as Nightingale [16].

Acknowledgments: This work was supported by the NASA OSIRIS-REx Participating Scientist program under a grant made to T. D. Glotch and A. D. Rogers. This material is based upon work supported by NASA under Contract NNM10AA11C issued through the New Frontiers Program. We are grateful to the entire OSIRIS-REx Team for making the encounter with Bennu possible.

References: [1] Clark, B. E. et al. (2011) *Icarus*, 216, 462-475. [2] Hergenrother, C. W. et al. (2013) *Icarus*, 226, 663-670. [3] Binzel, R. P. et al. (2015) *Icarus*, 256, 22-29. [4] Hamilton, V.E. et al. (2019) *Nature Astronomy*, *3*, 332. [5] Christensen, P. R. et al. (2018) *Space Science Reviews*, *214*(5), 87. [6] Ramsey and Christensen (1998) *JGR*,103, 577-596. [7] Rogers and Aharonson (2008) *JGR*, 113, E06S14. [8] Tucker, J. M. et al. (2010) *Chemical Geology*, 277, 137-148. [9] Dyar, M. D. et al. (2016) *American Mineralogist*, 101, 1171-1189. [10] Breitenfeld, L. B. et al. (2018) *American Mineralogist*, 103, 1827-1836. [11] Bland, P. A. et al. (2004) *Meteoritics & Planetary Science*, 39, 3-16. [12] Howard, K. T. et al. (2011) *Geochim. Cosmochim. Acta*, 75(10), 2735-2751. [13] King, A. J. et al. (2015) *Geochim. Cosmochim. Acta*, 165, 148-160. [14] Dyar, M. D. et al. (2012) *Spectrochim. Acta B*, 70, 51-67. [15] Clegg, S. M. et al. (2009) *Spectrochim. Acta B*, 64, 79-88. [16] Hamilton, V. E. et al. (2020) *LSPC, LI*, Abstract #1049.