AN INTEGRATED FINE AND COARSE PARTICULATE MACHINE LEARNING MIR MODEL PREDICTS MODAL MINERALOGY OF CI/CM CHONDRITIC ASTEROIDS AND BENNU. 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: CI and CM chondritic meteorites are composed of primitive materials that record early Solar System processes (e.g., aqueous alteration). Bennu, the target of the OSIRIS-REx spacecraft, is a near-Earth asteroid with a composition analogous to CI and/or CM chondrites [1]. Because asteroids like Bennu provide important information about the building blocks of the early Solar System, the development of methods for quantitative remote mineralogical analysis is desirable. Here we focus on constructing a mid-infrared (MIR) model for the prediction of fine and coarse particulate mineral abundances of CI/CM chondritic materials. The model can be applied to laboratory data, OSIRIS-REx Thermal Emission Spectrometer (OTES) data collected of Bennu, and infrared telescopic observations of other asteroids.

Bennu, an asteroid littered with boulders [2], has coarse particulate materials that contribute to OTES spectra. However, OTES spectra cannot be satisfactorily modeled only by coarse particulate mineral spectra, and Hamilton et al. interpreted a fine component contributing to OTES spectra [3]. Therefore, a further investigation of the contribution of fines is worthwhile. In the MIR, spectra of fine and coarse material have different characteristics (Figure 1). Additionally, fine particulate minerals contribute nonlinearly to spectra in mixture, complicating their quantification [4].

This work utilizes an integrated fine (<50 μm) and coarse (>125 μm) particulate MIR spectral library of mineral mixtures to create a machine learning partial least squares (PLS) multivariate analysis model. PLS machine learning multivariate analysis is an alternative approach to traditional linear models and removes the assumption of linear mixing across all wavelengths, allowing for the simultaneous modeling of fine and coarse particulate minerals.

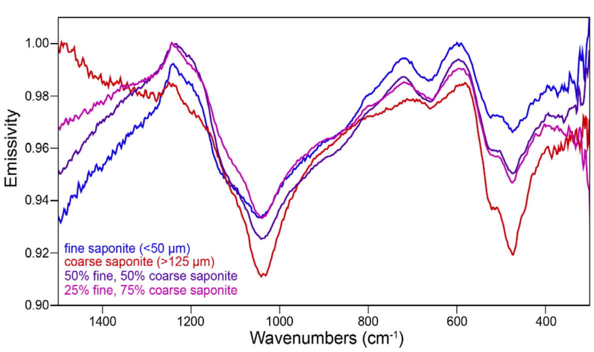

Figure 1. MIR SAE spectra of fine (<50 μm), coarse (>125 μm), 50% fine/ 50% coarse, and 25% fine/ 75% coarse particulates of the end-member saponite. All samples were darkened with 11 vol% carbon powder.

Sample Suite: The mineral species utilized in this work are terrestrial samples commonly present within CI and CM chondrites [5–8]. These minerals include antigorite, cronstedtite, saponite, magnetite, pyrrhotite, olivine (Fo_{40}, Fo_{80}, Fo_{95}), calcite, dolomite, ferrihydrite, gypsum, and enstatite. 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 and coarse particulates. Each sample was darkened with 11 vol% carbon powder to reduce the visible albedo, which partially controls the MIR spectra of materials collected in a simulated airless body environment [9].

The sample suite includes 13 end-members (as both fine and coarse particulates), 102 fine mineral mixtures, and 52 fine/coarse particulate mixtures. The end-member abundances of the 102 fine mineral mixture training set are summarized in Figure 2. Some of the mixtures act as analogs to CI and CM chondrites and match meteorite literature values [5–8]. Additionally, the model includes binary or ternary mineral mixtures. These mixtures are useful in broadening the mineral abundance range from 0 to 100 vol% for each mineral. This is necessary for the machine learning model because it allows for the prediction of unexpectedly high or low abundances by the model. In addition to the sample suite of real physical mixtures, 102 synthetic coarse sample spectra were made by linear combinations of coarse end-members.

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.

Multivariate Analysis: We utilized PLS multivariate analysis to build a model that can be

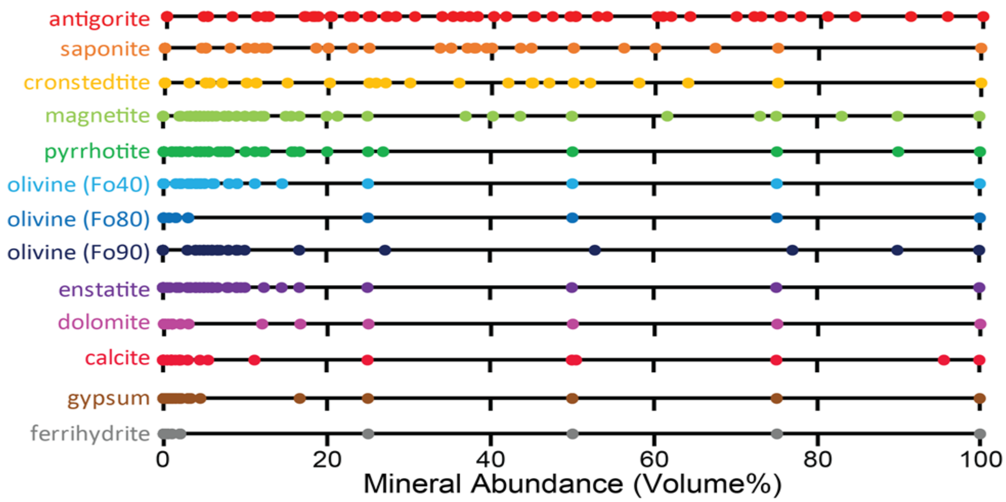

Figure 2. Mineral abundances of all mineral species for the training set of 13 end-members and 102 mineral mixtures. The 102 coarse linear mixtures mirror the abundances of the fine mineral mixtures.

applied to MIR data of meteorites or asteroids with CI- or CM-like compositions. The wavenumber range of the model used was 1500–1280 and 1200–330 cm^{-1} to exclude a feature centered at 1260 cm^{-1} associated with carbon powder in the samples. The preliminary model includes 223 spectra for the prediction of antigorite, saponite, cronstedtite, magnetite, pyrrhotite, enstatite, and olivine. These minerals had lower internal prediction error than the other species and are expected to be found in higher abundances in CI/CM material and therefore this first attempt utilized fewer end-members than available. The internal root mean square error (RMSE) of the model ranged from 2–7 vol%. Because we used 223 spectra, we selected 15 folds (square root of the number of spectra). The 15 folds allow for the

cross validation of the RMSE of ±7.4 vol% as an error metric for spectra outside the model (unseen data) instead of an internal RMSE.

Murchison and Essebi: Using the MIR PLS model, we predicted the mineral abundances of fine particulate samples of the meteorites Murchison and Essebi (Table 1) and compared the results to quantitative XRD data [6,7]. Here the model overpredicts magnetite and anhydrous minerals while underpredicting phyllosilicates.

The empirical uncertainty of predicting the mineral abundances of Murchison and Essebi is <15 vol% by mineral species. This uncertainty is comparable to linear unmixing of coarse particulate materials (~5–15%, [10]). This indicates that with further refinement of the PLS model, predictions of coarse and fine particulates on Bennu can be quantitatively estimated.

Table 1. Prediction of modal mineralogy (vol%) of Murchison and Essebi by MIR PLS and quantitative XRD.

Mineral	Murchison MIR PLS	Murchison Quantitative XRD [6]	Essebi MIR PLS	Essebi Quantitative XRD [7]
phyllo-silicate	53	72.5	61.4	74.5
magnetite	10.0	1.1	14.6	5.2
pyrrhotite	1.8	1.2	5.2	3.9
enstatite	9.7	8.3	0.0	2.1
olivine	30.6	15.1	17.9	14.1

Ongoing Work: The multivariate MIR PLS model will be further refined to include calcite, dolomite, ferrihydrite, and gypsum. Abundance predictions may change with the inclusion of additional end-members.

We will utilize the final model for mineralogy predictions of the OTES global average, type 1 and 2 spectra of Bennu [3]. Additionally, we will apply the model to regions of Bennu for modal mineralogy maps. We will also investigate in greater detail surfaces showing evidence for a greater proportion of fine particles, such as Nightingale, the site where the OSIRIS-REx spacecraft collected a sample of regolith, as well as other areas previously considered as possible sampling sites.

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References: [1] Hamilton, V.E. et al. (2019) *Nature Astronomy*, *3*, 332. [2] Lauretta et al. 2019. [3] Hamilton, V. E. et al. (2020) *LSPC, LI,* Abstract #1049. [4] Ramsey and Christensen (1998) *JGR*, 103, 577-596. [5] Bland, P. A. et al. (2004) *Meteoritics & Planetary Science*, 39, –16. [6] Howard et al. 2009. [7] Howard, K. T. et al. (2011) *Geochim. Cosmochim. Acta,* 75(10), 2735-2751. [8] King, A. J. et al. (2015) *Geochim. Cosmochim. Acta*, 165, 148-160. [9] Shirley, K. A. (2018). Doctoral dissertation, State University of New York at Stony Brook. [10] Hamilton, V. E., and Christensen, P. R. (2000) *J. Geophys. Res. Planets*, *105*(E4), 9717-9733.