RETRIEVAL OF COMPOSITIONAL ENDMEMBERS FROM MARS EXPLORATION ROVER ALPHA PARTICLE X-RAY SPECTROMETER OBSERVATIONS. N. T. Stein[1], R. E. Arvidson[2], J. A. O'Sullivan[2], D. V. Politte[2], J. Finkel[2], E. A. Guinness[2]. [1]California Institute of Technology, Pasadena, CA. nstein@caltech.edu. [2]Washington University in St. Louis.

Introduction: The Mars Exploration Rover (MER) Alpha Particle X-ray Spectrometer (APXS) is an arm-mounted instrument that performs in-situ measurements of the chemical composition of Martian soils and rocks [1]. Targets are sometimes covered by multiple APXS measurements whose fields of view (FOVs) contain several distinct compositional endmembers that can be identified and characterized using Pancam 13 filter spectra [2]. Several techniques can be used to retrieve composition estimates [3, 4] of Pancam-based spectral endmember locations by solving the non-invertible matrix equation

$$C(A + \delta A) = D + \delta D$$

where C is a spatial transfer function matrix that describes the relative abundance of each compositional endmember within each APXS FOV, D is a matrix of oxide weight percentages for each APXS measurement, and A is a matrix containing the endmember oxide weight percentages. Here we describe an iterative implementation of a log-likelihood function to determine endmember oxide abundances, which allows chemical characterization of sub-FOV-scale features.

Method: The APXS FOV describes the relative signal of scattered X-rays as a function of lateral distance from the detector center. For each measurement the FOV is approximated by projecting the APXS signal calibration curve for a given stand-off distance onto a digital elevation map (DEM) of the target. The sensor head is assumed to be nadir to the surface. Representative endmember spectra are determined using multispectral Pancam images (0.432 to 1.009 µm) of the area of coverage. Endmember maps are computed from the spectral similarity between Pancam image pixels and representative endmember spectra using the Sequential Maximum Angle Convex Cone (SMACC) tool in ENVI. The spatial transfer function is calculated as

$$C_{mn} = \sum_i \sum_j M_{ijm} I_{ijn}$$

where M is one of m spectral endmember maps and I is the relative intensity of a signal at endmember map location (i,j) for APXS measurement n. The transfer function provides an initial condition for the endmember phase abundances within each APXS FOV. The endmember composition matrix A is calculated using an iterative log-likelihood function with the assumption of Poisson-distributed data:

$$A_{ik} = \min_{\{a,c\}} \sum_i \sum_j I\left(D_{ij} \,||\, \sum_k A_{ik} C_{kj}\right) = \min_{\{A,C\}} \min_{\{P_{klij}\}} \sum_i \sum_j \sum_k I(D_{ij} P_{klij} || A_{ik} C_{kj})$$

The algorithm is subject to a non-negativity constraint. A_{ik} is constrained to sum to unity in order to ensure convergence. The transfer function and endmember composition matrices $C_{kj}^{(n)}$ and $A_{ik}^{(n)}$ are updated during each of N iterations as

$$P_{klij}^{(n)} \leftarrow \frac{A_{ik}^{(n)} C_{kj}^{(n)}}{\sum_{k'} A_{ik'}^{(n)} C_{kj'}^{(n)}}$$

$$A_{ik}^{(n+1)} = \frac{\sum_j P_{klij}^{(n)} D_{ij}}{\sum_{i'} \sum_{j'} P_{kli'j'}^{(n)} D_{i'j'}}$$

$$C_{kj}^{(n+1)} = \sum_i P_{klij}^{(n)} D_{ij}$$

in order to converge to the final endmember oxide weight percentage matrix $A^{(N)}$. The number of iterations typically exceeds $N = 10^4$, after which the I-divergence of the updated endmember solution coverges to a nearly constant value. Standard errors associated with APXS measurements are propagated through the unmixing algorithm.

Cook Haven Endmember Retrievals: The Opportunity rover was directed to Cook Haven for its 5th winter season [5]. Cook Haven is dominated by low-lying bright outcrops characterized by broken plates that contain partially soil-filled fractures (Fig. 1). Two rocks, Pinnacle Island (PI) and Stuart Island (SI), were excavated and overturned by the rover to reveal abnormally dark material. Pancam false color images and Microscopic Imager (MI) anaglyphs show that PI and SI are coated by dark material, and that PI contains a thin, bright coating over a fresh rock surface that was likely cleaved by one of Opportunity's wheels [5].

Five overlapping APXS observations were acquired for PI and four for SI. The FOV of each APXS observation was computed as a function of target topography and sensor stand-off distance. Relative abundance maps of Pancam-derived spectral endmembers for PI were determined for four endmembers termed 'dark coating', 'bright coating', 'rock', and 'dusty rock' (Fig. 2). PI was chosen because of its relatively pure endmember exposures determined by examining Pancam and MI data. The coatings were assumed to be optically thick to Pancam and APXS. Pancam-based spectral endmember abundance maps derived from linear unmixing were used with the APXS FOV to generate the *C* matrix. Trials using the five PI APXS observations and four spectral endmembers yielded insufficient accuracy due to the low number of APXS measurements relative to the number of endmembers, which makes it increasingly difficult to converge to a unique solution. Accuracy was improved with the addition of SI and nine Cook Haven bedrock and soil measurements as well as the combination of the rock and dusty rock endmembers into a single rock endmember due to their spectral similarity. The resulting endmember compositions are physically sensible, with the bright coating characterized by high Mg and S and moderate Mn, and the dark coating characterized by high Mn, Ca, and P relative to bedrock [5]. The rock endmember resembles the properties of nearby rocks that are not dust-covered such as Green Island (Fig. 3).

Conclusions and Future Work: The log-maximum likelihood method has been successfully implemented to determine endmember oxide abundances from Opportunity APXS observations. Work is underway to implement the method using APXS spectra rather than oxide weight percentages. The increased number of data points in the spectral domain (507 spectral energy bins vs. 16 oxide weight percentages) results in faster solution convergence, although care must be taken to account for spectral noise and other factors. Oxide abundances of resulting endmember spectra can be subsequently computed. Additional work is underway to demonstrate the unmixing algorithm using Curiosity rover APXS measurements.

References: [1] Gellert R. et al. (2006) *JGR: Planets.* 111. E02S05. [2] Bell J. F. et al. (2003) *JGR: Planets.* 108. 8063. [3] VanBommel S. et al. (2016) *X-Ray Spectrometry.* #2681. [4] VanBommel S. et al. (2016) *LPSC XLVII*, this conference. [5] Arvidson R. E. et al. *Am. Min.* In Review.

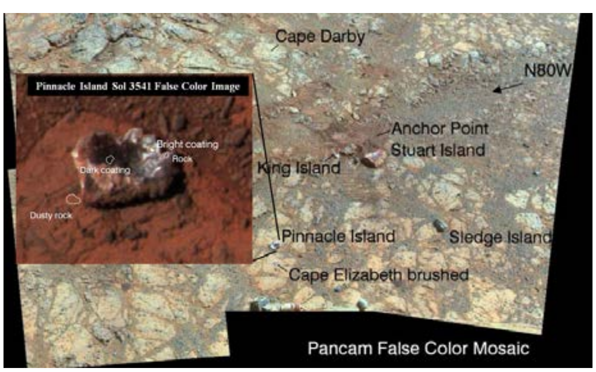

Figure 1: *Cook Haven and APXS targets used in spectral unmixing. Targets include Cape Darby, Cape Elizabeth, Pinnacle Island, Stuart Island, Green Island, Anchor Point, Sledge Island, Turnagain Arm, and Augustine. A false color Pancam image of Pinnacle Island shows the region of interest from which each endmember spectrum was collected.*

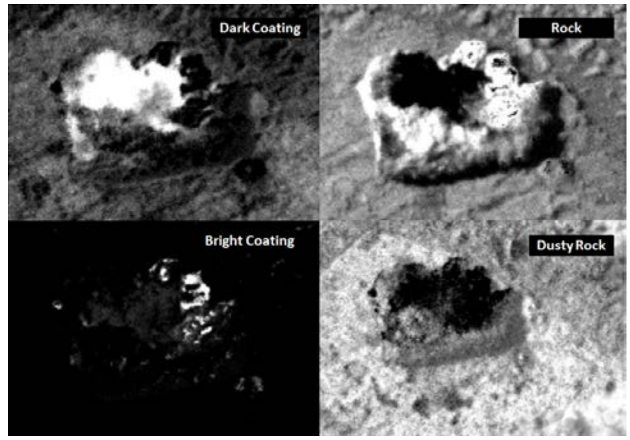

Figure 2: *Abundance maps of the four endmembers on Pinnacle Island. Each pixel has a fractional contribution from a different endmember defined using Pancam spectra.*

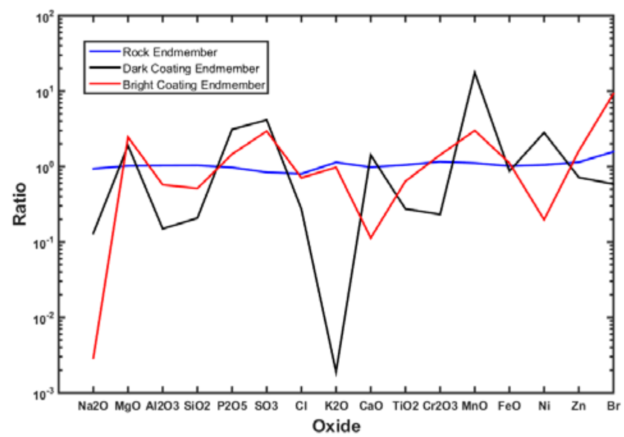

Figure 3: *Endmember oxide abundances ratioed to Green Island target, which was brushed using the Rock Abrasion Tool..*