ENHANCED CHARACTERIZATION OF THE MARS SCIENCE LABORATORY ALPHA PARTICLE X-RAY SPECTROMETER THROUGH ANALYSES OF SOFTWARE-SIMULATED SPECTRA.

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Introduction: The Alpha Particle X-ray Spectrometer (APXS) on the Mars Science Laboratory (MSL) rover *Curiosity* has conducted chemical analyses of over 700 targets in Gale Crater since landing in 2012. A thorough calibration was conducted pre-flight following the proven method of the Mars Exploration Rover (MER) APXS (e.g., [1]). The Earth-based calibration was conducted on powdered samples under ideal laboratory conditions. The resulting limits of detection (LOD) from this calibration are presented in [2].

The LOD for a given element depends on its abundance in the sample, the sample matrix composition, and experimental conditions. On Mars, experimental conditions are primarily controlled by (1) the placement of the APXS by a robotic arm (i.e., standoff), (2) the measurement duration, and (3) the temperature. Less-than-ideal standoff and thermal conditions occur in <5% of APXS targets due to unavoidable restrictions or tactical compromises in the positioning and/or timing of APXS measurements.

The spectral library of the MSL APXS was used to develop the "APXS Characterization by Empirical Simulation" (ACES) program [3]. The ACES program utilizes APXS spectra acquired on Mars to simulate a spectrum given defined experimental conditions and sample composition. The program also facilitates the input of multiple compositions (e.g., silicate bedrock + $CaSO_4$) to properly handle matrix effects.

Existing APXS-centric simulation software (e.g., [4, 5]) focuses on simulating peak areas on a computationally intensive photon-by-photon basis. The ACES algorithm avoids individual photon simulation. Thus, it is more computationally efficient and able to generate ~1,000 spectra per hour. As it is able to accommodate variable spectral conditions with high throughput, the ACES software package facilitates innumerable avenues of scientific inquiry [3]. Additionally, analyses of ACES simulated spectra offer insights leading to improved operational efficiencies on Mars.

Method: Spectra acquired on Mars were divided into "training" and "testing" categories. The former group was used to generate the predictive algorithms while the latter was used for confirmation. In the testing group, experiments executed on Mars specifically characterizing the APXS instrument's thermal and standoff (distance between sample and instrument) response were included. Each group had a broad range of compositions and experimental conditions.

Compositions and experimental conditions from measurements classified as "testing" were utilized as input for the ACES program. The corresponding simulated spectra were compared with the Mars-acquired original. The simulated spectra were also analyzed with the same APXS spectral analysis script that processes the spectra acquired on Mars.

Performance and Results: Simulated spectra from the ACES program provide the means to investigate the performance of the APXS in any number of conditions and compositions – an impossible feat to physically conduct in a terrestrial laboratory. An APXS spectrum is a superposition of signals that include X-rays germane to the atmosphere of Mars (e.g., [6]) as well as those from the APXS instrument itself. Figure 1 captures a simulated spectrum for the Mars target Ekwir_1_postbrush, acquired under ideal conditions. Characteristic lines from the sample are given in red, where peaks are associated with the lines of a given element (or elements). Figure 2 illustrates the agreement between the simulated Ekwir_1_postbrush spectrum (Figure 1) and the observed spectrum on Mars.
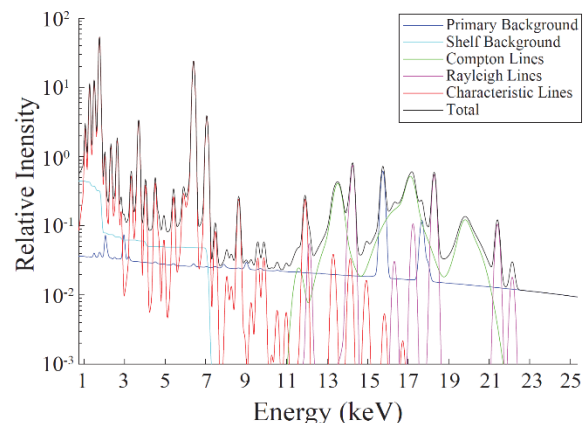
Figure 1: Simulated ACES spectrum illustrating the various contributions to an APXS spectrum. Characteristic lines (red) are sourced from the sample while scatter peaks (green, purple) correspond to inelastic and elastic scattered X-rays from the APXS sources. Background signals originate from within the APXS instrument, the Martian atmosphere, or are due to the APXS detector response. Figure from [3].

Simulated spectra remain in agreement as conditions deteriorate. Figure 3 compares a short-duration (4 minute) warm-temperature (+5°C) measurement of the MSL APXS calibration target with its ACES simulated counterpart. Zirconium (from the APXS collimator) and argon (from the atmosphere) peaks model accurately with variability in standoff (not plotted).
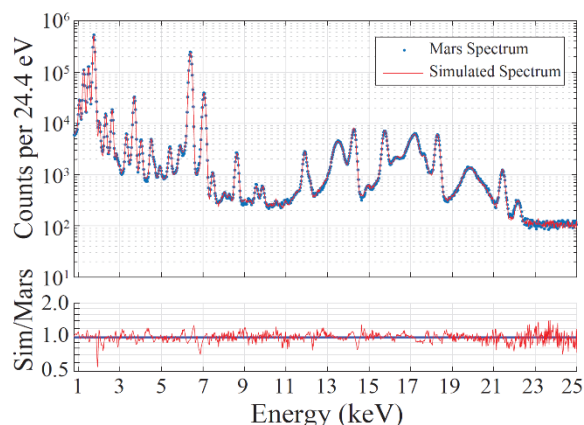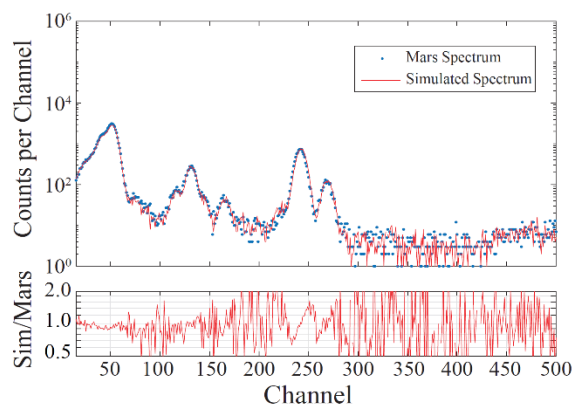

Figure 2: Simulated (red) and observed (blue) Ekwir_1_post-brush spectra, capturing program performance under ideal measurement conditions. Figure from [3].

The MSL APXS performance can be characterized by analyzing simulated ACES spectra. For example, peak errors for various elements in a typical Mars matrix at 0 cm standoff and ideal spectral resolution are a function of integration duration. Peak area uncertainty decreases rapidly with increasing measurement duration (Figure 4), especially for trace elements (e.g., Zn) and minor elements overlying a large background (e.g., Na). A peak area uncertainty of <5% is achieved after an hour of integration time with an ideal measurement configuration for the elements (excluding Ni and Br) reported to the public via NASA's Planetary Data System.

Ongoing Work and Future Applications: Applications of the ACES program include determining precise quantification limits (PQLs) for Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Rb, Sr, Y, and Pb as a function experimental conditions. Existing literature (e.g., [2]) offers the LOD for Ni, Zn, and Br under ideal conditions only. Situation-specific PQLs will benefit users of APXS data in the scientific community and better guide APXS tactical operations.

From a preliminary analysis of trace element PQLs as a function of experimental conditions, quantification of Cu, Ga, and Ge should be possible for Gale Crater soils. Potential local contributions will be investigated to better constrain the global component. PQL-focused studies of As, Se, Rb, Sr, Y, and Pb are planned after a

refinement to the high-energy (>11 keV) regime of simulated spectra. Investigations into the effects of multiple distinct chemical endmembers are also planned.

Figure 3: Comparison of simulated (red) and observed (blue) MSL APXS calibration target spectra acquired under non-deal (+5°C, 4 min duration) conditions. The comparison is truncated as scatter peaks are not displayed. Figure from [3].
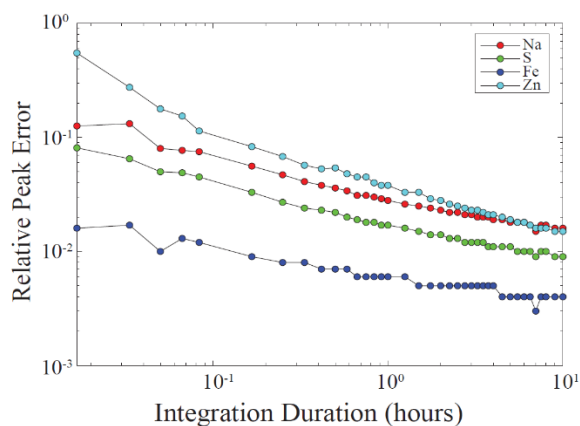
Figure 4: Peak area uncertainty in a typical Mars matrix with cold temperatures and the APXS deployed to contact. Figure from [3].

References: [1] Gellert et al., (2006), JGR, 111. [2] Gellert et al., (2015), Elements, 11. [3] VanBommel et al., (2019) NIM:B, 441. [4] Omand et al., (2005) NIM:B, 229. [5] Campbell et al., NIM:B, In Review. [6] VanBommel et al., (2018), JGR, 123.