ANALYSIS OF ACTIVE NEUTRON DATA FOR IN-SITU PLANETARY BULK GEOCHEMISTRY.
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Introduction: Active neutron spectrometers have been used extensively in Earth applications (*e.g.* in borehole/well logging analysis) to provide ~meter scale bulk geochemical information of rocks near the instrument. The Dynamic Albedo of Neutrons (DAN) instrument onboard the Mars Science Laboratory (MSL) Curiosity rover at Gale crater, Mars is the only such instrument deployed on a planetary body. Active experiments provide considerable advantages over traditional 'cosmic-ray' (passive) neutron experiments, albeit with a lifetime-limited neutron source. Given the high priority science targets currently traversed by Curiosity rover (*e.g.* Vera Rubin Ridge and the 'Clay unit') and future geologic units (*e.g.* the 'Sulfate unit'), it is critical that DAN continues to provide statistically robust geochemical constraints (*e.g.* bulk water content) and is readily utilized for tactical decision making (*e.g.* rapid identification of hydrated phases).

Using publicly-available data from MSL DAN [1], we investigate the effects of decreasing neutron generator output and provide solutions for maintaining sufficient uncertainty levels in current and future operational environments. We present a novel methodology for Bayesian analysis of active neutron data that provides a mapping of non-unique solutions and robust uncertainty quantification from random error and model noise. We also present data-driven analysis of DAN data for rapid assessment of anomalous rock geochemistries to allow for tactical decision making during operations and in future missions. This study provides several lessons learned for future active nuclear spectrometers deployed on planetary surfaces.

Neutron spectroscopy: In both active and passive neutron spectrometers, ~1-3 detectors accumulate neutron count rates across ~1-3 energy bins. For active detector systems the count rates are also acquired as a function of time after the pulse of a neutron source. This increases the number of variables that can be interpreted, as the time of arrival of neutrons is sensitive to several factors such as the depth of hydrated materials. In both passive and active techniques, low-energy neutrons provide important constraints on the abundance of neutron scatters (*e.g.* H) and neutron absorbers (*e.g.* Cl and Fe) in the substrate. The common passive, *i.e.* 'cosmic-ray', neutron spectrometers are often deployed at orbit and depend on the relatively low flux of Galactic Cosmic Rays (*e.g.* H^+) to produce neutrons in the subsurface; thus, they require long integration times and feature large sensing areas (>~100 km) when in orbit. Although active spectrometers must be deployed at the surface, requiring mobile platforms for widespread geochemical assay, they feature a neutron generator which allows for high signal-to-noise data and thus lower uncertainties. When paired with a gamma-ray detector, an even greater wealth of geochemical information is provided via time-resolved spectroscopy. In both cases, neutron spectrometers fill a 'gap' in geochemical remote sensing, as neutrons and gamma-rays penetrate to tens of centimeters, as compared to X-ray fluorescence (XRF) analyses which sense at microns depth, and radar which senses tens of meters to kilometers depth. Despite the many advantages of active neutron instruments, neutron generators are a lifetime-limited resource with variable output, introducing new complexities.

Non-unique solutions: Most detector packages provide count rates across 1-3 energy bins, yet planetary surfaces of unknown geochemistry can include variable abundances of many more than a few neutron scatters and absorbers, making the measurements inherently subject to degeneracy or non-unique solutions. Active neutron spectrometers overcome this limitation by producing time-resolved spectroscopy using pulses of high-energy neutrons and integrating the returned low-energy neutron counts across several time bins. This analysis allows for *additional degrees of freedom* and thus provides a more rich array of geochemical information from the instrument.

Dynamic Albedo of Neutrons Instrument: The Dynamic Albedo of Neutrons (DAN) instrument features a Pulse Neutron Generator (PNG) which produces 14.1 MeV neutrons across a <2 microsecond pulse through the following interaction:

$$^{2}D + {}^{3}T \rightarrow n\ (14.1\ MeV) + {}^{4}He\ (3.5\ MeV)$$

These high-energy neutrons interact with nuclei of several elemental species (*e.g.* H, Cl, Fe) and a proportion of the low-energy neutrons are detected. At manufacture, the PNG produced 1.34×10^7 neutrons per pulse [1] and its output has decreased over the lifetime of the instrument [2]. Due to the decrease in PNG output, the total instrument integration time has steadily increased; co-adding several measurements effectively provides longer integrations and thus recoups the effects of degradation to provide high signal-to-noise data. Through these operational adjustments, the PNG's functional lifetime (over 7 years) has far exceed its 3-year warrantied lifetime [1].

One aim of this work is to quantitatively define the relationship between the number of pulses and the level of uncertainty in the parameters (*e.g.* bulk water content). This is particularly useful as Curiosity rover traverses through a phyllosilicate-bearing unit [*e.g.* 3], where the robust characterization and quantification of H-rich minerals plays an important role in several hypotheses for the formation and diagenesis of Mount Sharp rocks [*e.g.* 4]. We also present ways in which strictly data-driven methods can be used tactically to inform decisions on short timescales, where statistical optimization may not be feasible. These investigations and lessons learned can be used in future investigations, *e.g.* DRAGNS on the Dragonfly spacecraft to the saturnian satellite Titan [5], where active neutron investigations will also be performed, or the passive neutron investigation on the NASA VIPER mission [6].

Methodology: Using publicly-available active DAN data hosted on the Planetary Data System (URL: https://pds-geosciences.wustl.edu/missions/msl/index.htm) we examine experiments across the rover traverse at drill sites where the geochemical and mineralogical abundances are well constrained from XRD and XRF analysis provided by the Chemistry & Mineralogy (CheMin) [7] and the Alpha-Particle X-ray Spectrometer (APXS) [8] instruments. We will investigate the relationship between the resulting uncertainties in the fitted parameters (*e.g.* bulk water content) to the PNG power from that epoch and the underlying geochemistry to project the required integration time for a given uncertainty threshold.

Markov chain Monte Carlo routine – In order to determine the range of good fit parameters for a non-linear active DAN instrument response, we developed a Markov chain Monte Carlo (MCMC) routine (also presented in [9] and [10]) based on the emcee, corner, and scipy packages for the Python Programming Language [11,12]. This statistical approach accounts for the non-gaussian uncertainty in geochemical parameters and provides a full mapping of the degeneracy (non-uniqueness) of solutions, provided a pre-existing modeling grid, *i.e.* a forward modeling approach. In Figure 1 we provide a sample output from our MCMC routine for active DAN experiments near the Highfield drill site at the Vera Rubin Ridge (VRR). The drilled rock features the presence of clays and a significant enrichment in Cl content; the latter is likely the source of high values for the macroscopic neutron absorption cross section (ξ_{abs}). Using this analysis we demonstrate that ***time-resolved neutron spectroscopy can constrain two free parameters uniquely with a single detector sensitive to E < 1 keV neutrons.***

Looking towards the future: The DAN instrument continues to perform in active mode with similar productivity to earlier epochs with minor changes to the operational procedures (longer integrations). We provide a path forward for obtaining robust uncertainty quantification in light of continued PNG degradation. Such advancements are necessary in characterizing the subsurface rocks of the clay unit currently traversed by Curiosity rover and the sulfate unit along the targeted path up Mount Sharp. Our statistical and data-driven approaches may also be useful in future active neutron flight instruments, particularly where there is minimal *a priori* information on the underlying geochemistry and where the nuclear spectrometer may be used for tactical decision making.

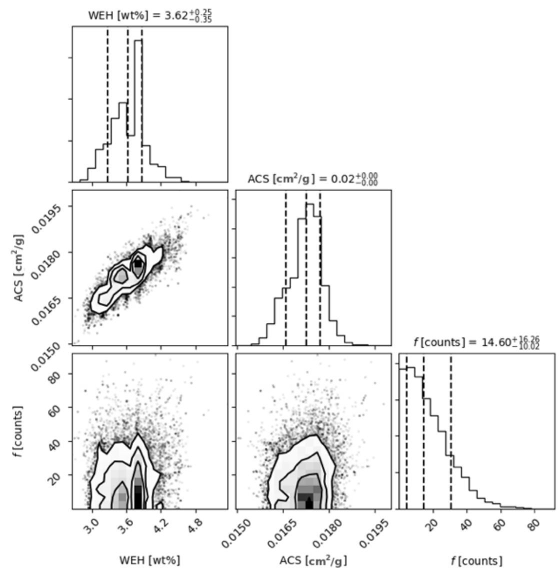

Figure 1 – Optimization for active DAN data near the ‘Highfield’ drill site (sols 2222-2245, site 73, drive 550, 48,000 PNG pulses in total). The 50th percentile values for bulk water content and macroscopic neutron absorption cross section are 3.62 wt% and 0.0017 cm^2/g.

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