Full spectrum fitting analysis of Bulk Elemental Composition Analyzer (BECA) gamma ray data. Mauricio Ayllon Unzueta[1,2], Bret Bronner[1], Frederic Gicquel[3], Jim Grau[3], Jeffrey Miles[3], Ann Parsons[1], Patrick Peplowski[4], Jeffrey Schweitzer[5], Richard Starr[1,6], James Zickefoose[7], [1]NASA Goddard Space Flight Center, Greenbelt, MD; [2]Universities Space Research Association, Columbia, MD; [3]Schlumberger Technology Corporation, Houston, TX; [4]Johns Hopkins University Applied Physics Laboratory, Laurel, MD; [5]University of Connecticut, Mansfield, CT; [6]Catholic University of America, Washington, DC; [7]Mirion Technologies Inc., Meriden, CT; (mauricio.ayllonunzueta@nasa.gov).

Introduction: The Bulk Elemental Composition Analyzer (BECA) is an instrument developed through NASA's Development and Advancement of Lunar Instrumentation (DALI) program to measure the *in situ* bulk elemental composition of the lunar regolith from either a lander or rover platform. BECA uses active neutron and gamma ray spectroscopy to make these measurements and thus consists of a Pulsed Neutron Generator (PNG) [1], a $CeBr_3$ scintillator Gamma Ray Spectrometer (GRS), and two He-3 neutron detectors. As shown in Figure 1, the PNG emits 14.1 MeV neutrons that induce lunar materials to emit gamma rays with energies characteristic of the elements that produced them. The GRS measures the energy spectra of these gamma rays to identify the elements present and establish their absolute concentrations in the regolith. The analysis of BECA's gamma ray spectral data yields quantitative elemental concentrations by mass (wt.%) in the material directly beneath the lunar lander or rover. A Compact Neutron Monitor (CNM) attached to the PNG precisely measures the output of 14.1 MeV neutrons to enable quantification of absolute elemental abundances.

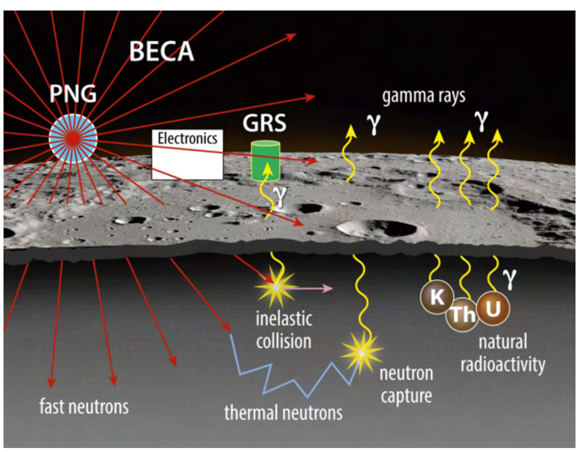

Figure 1: Illustration of BECA's main components and elementary physical principles of operation. Note that the neutron detectors are not shown.

BECA operations: The PNG's neutrons interact with nuclei in the lunar regolith primarily via two different nuclear processes: neutron capture (slow) and inelastic scattering (fast). The pulsed properties of the PNG allow for the independent spectral analysis of the gamma rays from these processes, which in turn provides a more detailed and complimentary analysis of the bulk elemental composition.

Full spectrum fitting is the most appropriate gamma ray spectral analysis technique for BECA, given the limited energy resolution of the $CeBr_3$ GRS. Rather than measuring the counts in individual gamma ray spectral lines, a weighted least squares fit is performed on the 0.7 - 10 MeV gamma ray spectrum as a whole to produce a linear combination of individual spectral components whose coefficients can then be converted to elemental concentrations.

As part of the design of such an instrument, Monte Carlo simulations of neutron and gamma transport have become essential to understand the elemental sensitivities for a given geometry, surface composition, and measurement times. For such purposes, we have developed an analysis routine based on weighted least-squares (WLS) full-spectrum fitting that will guide us through the instrument design process.

The ultimate goal of the analysis is to determine the elemental composition of an unknown sample of lunar regolith. However, the initial step towards achieving this goal is to test this analytical method against a sample that has been assayed by other means. In our case, we performed relevant experiments with a lunar surface simulant, which is a monument of Columbia River basalt that has been independently chemically assayed. The monument is located at a dedicated testing facility at Goddard Space Flight Center (GSFC) [2]. Consequently, in this presentation, we will show the results of the WLS fitting technique aided by Monte Carlo simulations together with its experimental benchmark.

Full-spectrum fitting technique: The code Monte Carlo N-Particle (MCNP) [3,4], which was developed and is maintained at Los Alamos National Laboratory (LANL), is used to simulate the neutron transport and interactions that result in gamma ray production throughout a defined 3D geometry.

Based on the above simulations, we can estimate the statistical uncertainty of the elemental concentrations that can be measured by spectroscopy.

These uncertainty values can also be converted into an acquisition time required to achieve a target statistical precision on each of the elements. Below, we briefly outline the procedure and will discuss its corresponding outcome.

1) The WLS solution (in matrix algebra) for the spectral yields (y) is as follows:

$$y = (S^T W S)^{-1} S^T W u$$

Where W is the weighting matrix containing the inverse variance of each channel, S is the matrix of the normalized standard spectra for each element obtained by simulations (as shown in Figure 2), and u is the total spectrum (the spectrum that is actually measured or simulated). Note that the spectral yield y is defined as the fraction of the total spectrum associated with each spectral standard.

2) The uncertainty of the relative yields (δy) for element j and total counts N is as follows:

$$\delta y_j = \frac{1}{\sqrt{N}} \sqrt{C_{jj}}$$

Where C is the covariance matrix of the solved yields.

3) Finally, the estimated uncertainties (δw) of the elemental weight concentrations are:

$$\delta w = k \delta y$$

Where k is a multiplicative factor that includes both an individual elemental spectral sensitivity and a general normalization factor that depends on the experimental environment [5].

Based on this analysis, we will discuss the estimated uncertainties of the elemental concentrations for our specific case scenario.

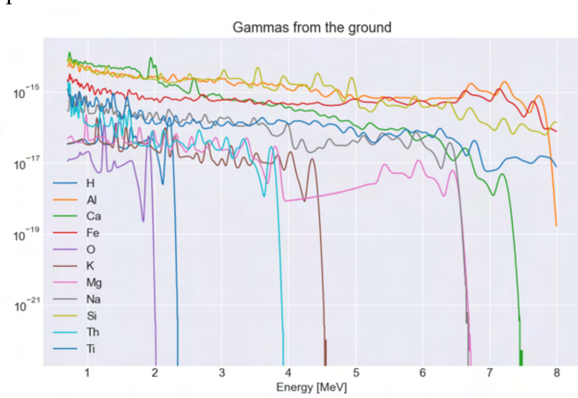

Figure 2: Simulated gamma ray standard spectra for each individual element in the overall surface composition. They constitute the S matrix in the equations above.

Experimental results: In order to provide experimental validation of the analytical procedure above, we performed an experiment at the Gamma-ray and Neutron Test Facility (GNTF) at GSFC consisting of a basalt monument (182.9 cm x 182.9 cm x 91.44 cm), a non-flight Thermo Fisher PNG (model MP 320), and a $CeBr_3$ detector (5.1 cm x 5.1 cm cylinder), as shown in Figure 3. Aluminum and high-density polyethylene were added to simulate a lunar rover and to artificially introduce moderating material to allow for a better measurement of neutron capture processes. A detailed simulation of this setup was performed and the results will be discussed in the context of the WLS analysis detailed above.

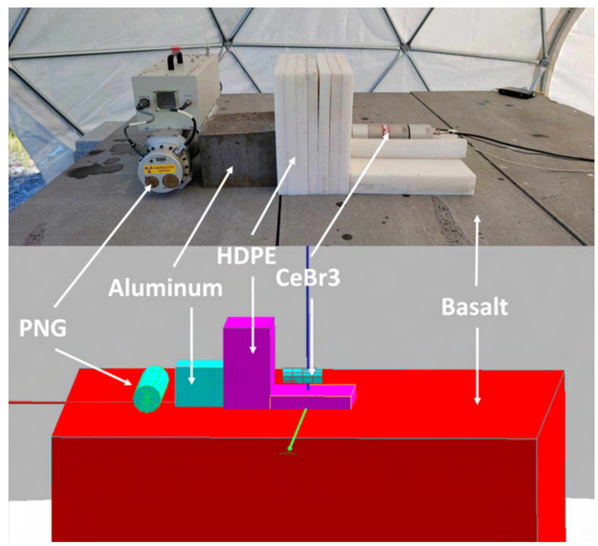

Figure 3: Experimental setup and its corresponding simulated geometry.

Note that even though this instrument is specifically designed for use on the lunar surface, it can easily be adapted to explore other moons, planets, or asteroids in our solar system such as Saturn's moon Titan [6].

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References: *[1] R. J. Radtke et al., SPWLA 53rd Ann. Logging Sym., 2012; [2] Parsons et al., IEEE Aerospace Conference, 2013, pp. 1-11; [3] Goorley et al., Nuclear Technology 180, 298-315, 2012; [4] Werner, et al, MCNP Version 6.2 Release Notes, 2018; [5] J.A. Grau et al., Nucl. Geophys, Vol. 3 No. 4, pp. 351-359.; [6] E. P. Turtle et al., 50th LPSC, #2888, 2019.*