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Development of a surrogate model for elemental analysis using a natural gamma ray spectroscopy tool

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HIGHLIGHTS

- A novel computational model for efficiently computing elemental standards for varying borehole conditions has been developed.
- A model of an experimental test pit was implemented in the Monte Carlo code GEANT4 for computing elemental standards.
- A surrogate model was developed that is based on fitting a semi-empirical model to GEANT4 computed spectra at various casing and cement thicknesses within the borehole.
- Future work will involve case studies and an extension of the Monte Carlo computed elemental standards to a variety of nuclear logging tool designs.

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ABSTRACT

A systematic computational method for obtaining accurate elemental standards efficiently for varying borehole conditions was developed based on Monte Carlo simulations, surrogate modeling, and data assimilation. Elemental standards are essential for spectral unfolding in formation evaluation applications commonly used for nuclear well logging tools. Typically, elemental standards are obtained by standardized measurements, but these experiments are expensive and lack the flexibility to address different logging conditions. In contrast, computer-based Monte Carlo simulations provide an accurate and more flexible approach to obtaining elemental standards for formation evaluation.

The presented computational method recognizes that in contrast to typical neutron–photon simulations, where the source is typically artificial and well characterized (Galford, 2009), an accurate knowledge of the source is essential for matching the obtained Monte Carlo elemental standards with their experimental counterparts. Therefore, source distributions are adjusted to minimize the L2 difference of the Monte Carlo computed and experimental standards. Subsequently, an accurate surrogate model is developed accounting for different casing and cement thicknesses, and tool positions within the borehole.

The adjusted source distributions are then utilized to generate and validate spectra for varying borehole conditions: tool position, casing and cement thickness. The effect of these conditions on the spectra are investigated and discussed in this work.

Given that Monte Carlo modeling provides much lower cost and more flexibility, employing Monte Carlo could enhance the processing of nuclear tool logging data computed standards.

1. Introduction

As an essential part of drilling and evaluation, nuclear well logging provides important parameters such as porosity, bulk density and lithology/mineralogy that help to understand and evaluate the formation (Ellis and Singer, 1987). A few examples of nuclear log types are the natural gamma ray, gamma-ray density, neutron porosity, and pulsed-neutron instruments.

Common among these methods is that the characteristic transport of particles, neutrons (n) or photons (p), through the formation is used to determine typical formation parameters and/or its composition. The transport of particles in a host medium is governed by the neutron transport equation (Duderstadt and Hamilton, 1976):

$$\vec{\Omega}\nabla\psi\left(r, \vec{\Omega}, E\right) + \sigma_t\psi\left(r, \vec{\Omega}, E\right) = \int_0^\infty dE' \int_{4\pi} d\vec{\Omega}'\, \sigma_s\left(r, E', \vec{\Omega} \to E, \vec{\Omega}\right)\psi\left(r, \vec{\Omega}', E'\right) + S\left(r, \vec{\Omega}, E\right), \quad (1)$$

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where the independent variables r: space, E: energy, and $\vec{\Omega}$: direction are given. The dependent variable is the angular flux denoted by ψ that is driven by the distributed source S. Further, the total interaction cross section σ_t and the double differential scattering cross section $\sigma_s\left(r, E', \vec{\Omega} \rightarrow E, \vec{\Omega}\right)$ are material properties that characterize the transport's host material. In addition to Eq. (1) suitable boundary conditions are given on the inflow boundary. Typically, well logging problems feature vacuum (no inflow) boundary conditions. For the further development of this work it is noteworthy that the particle transport equation is linear and therefore the principle of superposition holds.

Typically, well-logging applications utilize a detector and its response R is used for drawing conclusions about the formation. Mathematically the response is given by:

$$R(E) = \int_{4\pi} d\vec{\Omega} \int_0^{\infty} dE' T(r, \vec{\Omega}, E' \rightarrow E)\psi(r, \vec{\Omega}, E'), \quad (2)$$

where T is the detector response function.

For the mathematical solution of the transport equation Monte Carlo methods are considered to be the most accurate method available especially in the presence of complicated geometries. Monte Carlo methods have been widely employed in the optimization of nuclear logging tool design, simulation, benchmark and the development of interpretation methods for following reasons:

1. Monte Carlo simulations are an inexpensive and time-saving method for optimizing the design of new logging tools. Key design parameters include detector type, detector position, detector size, detector shielding, effect of housing materials on the response of the tool, and so forth.
2. Once a tool has been designed, Monte Carlo simulations are a cost-effective method to simulate changing borehole environments that will be encountered during logging. These data can be used to develop environmental correction algorithms for the tool. Parameters that might be studied include: hole size, casing size and weight, lithology, porosity, borehole fluid types and saturations, formation fluid types and saturations, clay content, invasion fronts, cement types, etc.
3. Another use of Monte Carlo simulations is to improve the understanding of the tool's response. Often, this can be accomplished by modifying the code to provide additional information such as elemental standards or the depth-of-investigation of the measurement.

In the scope of this work, we focus on one specific application of Monte Carlo modeling in nuclear well logging: obtain elemental standards for formation evaluation using a natural gamma ray spectroscopy tool.

The first spectroscopy tool detecting natural radioactivity in subsurface formations is introduced in the late 1930s (Ellis and Singer, 1987). Since then, the natural gamma ray spectroscopy tool has been operated in different formations, e.g. carbonate, sandstone, and shale, around the world to provide geological data to determine where layers of shale or oil-bearing rock exist.

The spectroscopy tool measures the natural gamma radiation ranging from below 0.1 to well above 3.5 MeV. Natural gamma ray radiation is a high-energy electromagnetic wave that originates mainly from three sources: K-40 isotope; Th-232 and U-238 decay series. Measuring the gamma ray signature of a formation can identify the quantities of the three natural radioisotopes present in the formation. To achieve an accurate assessment of isotope quantities as well as lithology and mineralogy, a set of accurate elemental standards for various isotopes is critical. This is because elemental standards are used as parameters to solve the least square problem related to the spectra unfolding (Pemper et al., 2006).

In general, elemental standards are defined as the signals that a detector obtains from a formation that only consists of a single gamma-ray emitting element. Traditionally, elemental standards are obtained through test-pit experiments, which are both time-consuming and expensive. This methodology predates the advent of accurate and efficient modeling capabilities of particle transport. The experiments allow one to obtain elemental standards for a single normed case without understanding or accounting for the variability of borehole conditions. Particularly, it is exceedingly difficult to obtain a series of different elemental standards each of which caters to a specific scenario through experiments. Therefore, Monte Carlo modeling provides an alternative approach that enables us to obtain elemental standards in an efficient manner of great flexibility and accuracy.

In general, the analyst is interested in highly customized situations with different borehole conditions, borehole diameter, casing and cement layer thicknesses etc., have to be considered. These conditions impact the effective elemental standard such that in principal the Monte Carlo model would have to be rerun for each case to obtain an accurate elemental standard. Even though Monte Carlo models are more efficient than experimental evaluation of customized elemental standards, its evaluation would still require several hours of computing time (up to possibly one day of computing time on a desktop computer). This work suggests a surrogate model based in Monte Carlo generated data that accurately captures the effect of varying borehole conditions. The evaluation of this surrogate model takes of the order of split seconds. It will be demonstrated that the constructed surrogate model provides an extraordinary level of accuracy.

The paper is organized as following: Section 2 introduces the structure of the test pit, from which the experimental elemental standards are measured; Section 3 describes the procedure of Monte Carlo modeling using GEANT4 code; 13Section 4 compares two sets of elemental standards obtained from test pit and Monte Carlo modeling; in Section 5, a field log case is presented and analyzed using both sets of standards. Section 6 summarizes this work and discusses future research.

2. Elemental standards measured at test pit

The elemental standards U (Uranium), Th (Thorium), K (Potassium) for the natural gamma ray spectroscopy tool are obtained at the API test pit facility located at the University of Houston. Pits have been designed and built for calibrating natural gamma ray spectroscopy logging instruments. Sketches of the K-U–Th calibration facility are shown in Figs. 1 and 2 (Arnold, 1982).

The facility consists of two cylindrical forms each 7.75 feet in diameter, set in activity concrete within bored holes and sealed from the surrounding formation. The overall depth of the pits is 30 feet with 15-feet ratholes on each borehole. Each pit contains a series of poured layers or zones of “barren” cement and layers of similar cement into which known amounts of K, U, and Th and mixtures of K, U, and Th have been added. Calculations have shown that zones 5 feet thick will appear essentially “infinite” in vertical extent to a 12-in. long gamma ray detector instrument centered within the zone. Each cement zone was constructed in a single pour. Each pit contains three vertical boreholes with diameters of 6 in., 8 5/8 in., and 12 in.. Each borehole extends below the bottom of the pit into a rathole approximately 15 feet deep (RP31A, 2005; $author1$ et al., API).

The arrangement of the boreholes is illustrated in Figs. 1 and 2. Calculations show that the distance between boreholes and between any borehole and the periphery of the model is large