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**Physics and Rapid Forward Modeling of Logging-While-Drilling
Neutron-Gamma Density Measurements**

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**Physics and Rapid Forward Modeling of Logging-While-Drilling
Neutron-Gamma Density Measurements**

by

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À mon grand-père,

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Physics and Rapid Forward Modeling of Logging-While-Drilling Neutron-Gamma Density Measurements

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Although radioactive chemical sources have long been used in borehole nuclear tools for in-situ porosity estimation, they pose non-negligible health, safety, and environmental risks. Pulsed neutron generators were successfully introduced as replacements for americium-beryllium (AmBe) sources in neutron-based measurements. However, bulk density is still generally measured using Gamma-Gamma density tools operating with cesium-137 sources.

Neutron-activated gamma-ray measurements (Neutron-Gamma) are a safer alternative to Gamma-Gamma density measurements because cesium-137 is replaced with a pulsed neutron generator. Thereafter, bulk density is estimated from neutron-induced non-capture gamma-ray counts corrected for neutron transport. Field studies with commercial Neutron-Gamma density tools revealed several practical limitations, including sensitivity to borehole conditions and decreased accuracy in high-density formations, shales, and shaly formations. The main purpose of this dissertation is to develop new measurement and interpretation procedures to mitigate such limitations.

With the objective of accurately capturing the measurement physics, I designed a new theoretical, albeit realistic logging-while-drilling (LWD) Neutron-

Gamma density tool. This new tool combines inputs from two gamma-ray detectors and two fast neutron detectors to deliver density accuracies that favorably compare to those obtained with traditional Gamma-Gamma density measurements, i.e., 0.013 g/cm³ in shale-free formations, and 0.019 g/cm³ in shale and shaly formations. Similar to other nuclear measurements, Neutron-Gamma density is affected by bed-boundary and layer-thickness effects that can mask the true formation bulk density when implementing conventional interpretation methods. Borehole environmental effects are additionally mitigated using empirical corrections because “spine-and-rib” compensation is impractical. However, for standoff values greater than 0.63 cm (0.25 in), such empirical corrections should be avoided as they no longer remain independent of formation properties.

Three-dimensional geometrical and borehole effects can be mitigated using fast numerical simulations coupled with inversion-based interpretation. To simulate borehole LWD Neutron-Gamma density measurements, I developed a fast-forward modeling algorithm based on first-order approximations and flux sensitivity functions. The algorithm is over 500,000 times faster than industry-standard Monte Carlo methods and achieves root-mean-square errors of less than 1% (0.023 g/cm³) in formations with spatially complex geometry, including high-angle wells, thinly-bedded formations, and invaded beds. However, fast numerical simulations based on first-order approximations have limited accuracy when modeling borehole environmental effects. The Neutron-Gamma density fast-forward algorithm can improve the interpretation of measurements when standoff is less than 1.27 cm (0.5 in). Conversely, for larger values of standoff, spatial flux perturbations give rise to higher-order measurement responses that are not

captured with first-order approximations, yielding density errors of up to 0.04 g/cm^3 for 2.54 cm (1 in) standoff.

The second part of this dissertation introduces new methods to improve borehole environmental corrections of nuclear measurements based on single-particle transport. They rely on higher-order rapid forward simulations wherein sensitivity flux perturbations are quantified using approximations to the Boltzmann transport equation. For neutron measurements, the diffusion flux-difference method is enhanced with a two-step algorithm that minimizes the size of the perturbation and yields average errors of 1 porosity unit (p.u.) in boreholes with up to 2.5-cm (1-in) standoff. For Gamma-Gamma density measurements, the gamma flux-difference (GFD) method is introduced to quantify gamma-ray flux perturbations using exponential point kernels and a Rytov approximation. This latter procedure yields maximum density errors of 0.02 g/cm^3 in boreholes with up to 4.44 cm (1.75 in) standoff. The methods developed in this dissertation represent the first step toward future improvements in fast modeling of borehole environmental effects for nuclear measurements based on coupled neutron and gamma-ray transport, such as Neutron-Gamma density.

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Chapter 1: Introduction

This introductory chapter reviews the literature relevant to this dissertation, outlines the research objectives, and summarizes the findings of the subsequent chapters.

This dissertation is composed of two technical sections. The first section introduces new measurement and interpretation procedures for Neutron-Gamma density logging tools. The second section focusses on developing fast-forward modeling algorithms to simulate and mitigate borehole environmental effects in nuclear measurements.

1.1 LITERATURE REVIEW

1.1.1 In-situ Porosity Estimation with Neutron and Gamma-Gamma Density Measurements

Borehole nuclear measurements are fundamental to estimating in-situ porosity and identifying fluids in formation evaluation. Neutron-porosity tools traditionally operate with radioactive americium-beryllium (AmBe) sources (Ellis and Singer, 2007). These tools generate high-energy neutrons that deposit their energy within the formation, primarily through elastic scattering with hydrogen nuclei. Neutron measurements are thus sensitive to the hydrogen index (HI) of the formation (i.e., the amount of hydrogen within the formation) and can be combined with bulk density measurements to estimate formation porosity.

Bulk density is traditionally measured with Gamma-Gamma density logging tools that use cesium-137 chemical sources to generate 0.662-MeV (megaelectron volt) gamma-rays at a constant rate and at a fixed distance from the detectors. At these energy levels, Compton scattering is the dominant interaction and pair production is non-existent. Furthermore, gamma-ray attenuation is proportional to the electron density of the formation (in agreement with the fundamental law of gamma-ray attenuation, Ellis and Singer, 2007), where electron density is linearly correlated with bulk density. Bulk density is generally measured at long- and short-spaced gamma-ray detectors with an average accuracy of 0.015 g/cm³.

In enlarged boreholes, nuclear measurements should be corrected for borehole environmental effects, such as standoff and mud composition. Standoff is defined as the distance between the external diameter of the logging tool and the borehole wall. When the logging tool is centered in the borehole, standoff is constant; however, when the logging tool is not centered, standoff varies azimuthally. For Gamma-Gamma density measurements, borehole environmental effects can be mitigated using the “spine and rib” compensation method where no a-priori information about standoff or mud density is required. The basis for this technique is that the sensitivity of bulk density measurements to standoff varies depending on detector spacing (Wahl et al., 1964).

1.1.2 Neutron-Gamma Density Measurements

Radioactive chemical sources pose health, security, and environmental risks, as well as significant handling, storage, transportation, and disposal costs (Aitken et al., 2002). Despite numerous regulatory requirements (Aitken et al., 1994), there have been cases of nuclear sources being breached, stuck downhole,

and lost (Badruzzaman et al., 2009). Therefore, limiting the use of radioactive chemical sources is a high priority for the oil industry (Weller et al., 2005).

Pulsed neutron generators offer enhanced safety benefits because they can be switched on and off to generate 14.1-MeV neutrons. They have been successfully implemented for wireline and logging-while-drilling (LWD) borehole neutron measurements as an alternative to chemical AmBe sources.

Replacing cesium-137 sources in Gamma-Gamma density tools is much more challenging. One possible solution is to use an electron linear accelerator (LINAC) to generate bremsstrahlung X-rays. Although King et al. (1987) developed one such experimental system, LINAC sources have not been employed by any commercial logging tool, suggesting that practical implementation is extremely difficult. Conversely, Neutron-Gamma density measurements are another possible solution that has been successfully implemented in a commercial logging tool (Evans et al., 2012; Reichel et al., 2012).

For Neutron-Gamma density measurements, cesium-137 is replaced by a pulsed neutron generator, which reduces the radiation risk for tool operators and the environment (Weller et al., 2005). Bulk density is estimated using neutron-activated secondary gamma rays, a concept first introduced by Wilson (1995). The secondary gamma-ray source is distributed within the formation. Therefore, gamma-ray counts respond to formation electron density, but they are also affected by formation properties that govern neutron transport, such as hydrogen index. The first applications, which were for measurements acquired behind casing, used gamma rays generated by fast neutrons, referred to as inelastic gamma-rays (Odom et al., 1994, 1997; Neuman et al., 1999). Capture gamma-

rays, emitted by the radiative capture of thermal neutrons, were excluded from the measurement because thermal neutron transport is highly sensitive to hydrogen index.

Despite the improvements gained by using inelastic gamma-rays, the measurement remained sensitive to hydrogen index variations, which led to new designs that incorporated neutron detectors to correct for neutron transport. Odom et al. (2001) introduced a through-casing Neutron-Gamma density tool with one fast neutron detector. Later, the first commercial Neutron-Gamma density tool, developed by Evans et al. (2012) and Reichel et al. (2012), made use of thermal and epithermal neutron detectors. Nonetheless, field studies with the commercial LWD Neutron-Gamma density tool (Majidi et al., 2012; Atfeh et al., 2013; Alakeely and Meridji, 2014; Kyi et al., 2014; Mahiout et al., 2016) revealed several practical limitations compared with traditional Gamma-Gamma density measurements, including elevated sensitivity to borehole conditions (because the measurement is uncompensated, i.e., bulk density is estimated at a single detector) and decreased accuracy in high-density formations, shales, and shaly formations.

1.1.3 Fast Modeling of Borehole Nuclear Measurements

The coupled Boltzmann transport equation describes neutron and gamma ray transport processes. This equation can be solved deterministically using numerical methods in simple geometries (Bertozzi et al., 1981; Lewis and Miller, 1984;) or using simplifying assumptions, such as the diffusion approximation for thermal neutrons (Tittle, 1961). However, in complex three-dimensional geometries, accurate modeling requires the use of Monte Carlo (MC) algorithms, such as MCNP (Monte Carlo N-Particle code, Goorley, 2014). The probabilities of

transport and interaction between millions of particles are calculated individually to evaluate detector counts based on the law of large numbers. Therefore, while highly accurate, MCNP is computationally expensive and impractical for the simulation (and inversion) of borehole nuclear measurements over long depth intervals.

Sensitivity functions, which were introduced by Watson (1984, 1992), Couët and Watson (1993), and Case et al. (1994), led to the development of rapid and accurate fast-forward modeling algorithms. Flux sensitivity functions (FSFs) are computed using a modified version of MCNP (Mendoza et al., 2007) that takes advantage of the importance calculations performed with its forward-adjoint generator (Booth and Hendricks, 1984). Mendoza et al. (2007) showed that numerical simulation algorithms based on FSFs and first-order perturbation theory (Lewins, 1965; Greenspan, 1976) were accurate, reliable, and computationally efficient in diverse logging environments. In addition, they also developed a Linear Iterative Refinement (LIR) method to select the optimal FSF at each measured depth using iterative linear interpolations between base-case sensitivity functions that are precalculated with MCNP. Fast-forward algorithms based on the LIR method were developed for Gamma-Gamma density (Mendoza et al., 2010a), neutron porosity (Mendoza et al., 2010a), Sigma (Ortega et al., 2014), and spectroscopy (Ajayi et al., 2015a) borehole nuclear measurements. Additionally, these algorithms were successfully implemented with inversion-based interpretation procedures (Sanchez-Ramirez et al., 2009; Heidari et al., 2012, 2013; Ijase et al., 2013b, 2014; Ajayi et al., 2015b; Ortega et al., 2017).

Higher-order effects, in the form of sensitivity flux perturbations, arise in zones with properties that contrast significantly, such as at invasion fronts, the borehole wall, or some bed boundaries. Throughout this dissertation, higher-order effects refer to effects that cannot be accounted for using the first-term of a Taylor series expansion. Because such effects cannot be accurately simulated using first-order perturbation theory, Zhou et al. (2009), Mimoun et al. (2011), and Ijase et al. (2013a) developed fast-forward algorithms based on higher-order approximations. For Gamma-Gamma density measurements, Zhou et al. (2009) introduced a second-order fast-forward model based on first and second-order sensitivity functions. The sensitivity functions were calculated with grid-by-grid perturbations using a perturbation feature available in MCNP. Then, Mimoun et al. (2011) implemented one-dimensional (1D) diffusion approximations to quantify flux perturbations along the vertical direction for Sigma measurements. For neutron measurements, Ijase et al. (2013a) introduced the diffusion flux-difference method to quantify 3D flux perturbations using one-group neutron diffusion approximations.

1.2 PROBLEM STATEMENT

1.2.1 Section I: Neutron-Gamma Density Measurements

Inanc (2014) studied the fundamental physical differences between Neutron-Gamma density and Gamma-Gamma density measurements. He raised two valid concerns regarding the use of neutron-induced gamma-rays for the estimation of bulk density. First, the secondary gamma-ray source is distributed within the formation and varies with formation properties in space, energy, and

intensity. Second, gamma rays are generated at higher-energy levels, which implies that pair production interactions are no longer negligible. Inanc (2014) concluded that Neutron-Gamma density measurements are sensitive to formation properties other than electron density and are therefore likely to require highly complex interpretation procedures.

The commercial Neutron-Gamma density tool developed by Evans et al. (2012) and Reichel et al. (2012) has a relatively low density accuracy compared with Gamma-Gamma density measurements: 0.025 g/cm³ in clean formations and 0.045 g/cm³ in shales. Such errors in the estimation of bulk density are caused by variations in the secondary gamma-ray source (in space, energy, and intensity) that are not fully captured by the tool design. Density accuracy is lower in shales than in shale-free formations because shales exhibit complex mineralogy that translates into increased variability in the secondary gamma-ray source. Complex minerals are composed of certain elements such as aluminum (Al), chlorine (Cl), iron (Fe), and magnesium (Mg) whose elastic, absorption, and inelastic cross sections exhibit higher variability than oxygen (O), carbon (C), or calcium (Ca) between 1 and 14.1 MeV. Another limitation of Neutron-Gamma density measurements was revealed by field studies (Mahiout et al., 2016): Neutron-Gamma density is very sensitive to standoff effects because the measurement is uncompensated.

To the best of the author's knowledge, there has been no previous attempt to investigate the physics of Neutron-Gamma density measurements and optimize the tool design for the purpose of maximizing density accuracy across formations with complex mineralogy.

1.2.2 Section II: Fast-Modeling of Borehole Environmental Effects in Nuclear Measurements

Borehole environmental effects are traditionally mitigated with compensation algorithms, such as the “spine and rib” technique for Gamma-Gamma density measurements (Wahl et al., 1964), and dual-spacing compensation methods for neutron measurements (Alger et al., 1972). However, for more complex borehole nuclear measurements, including Neutron-Gamma density and spectroscopy, such compensation procedures become impractical. Instead, empirical borehole environmental corrections are applied, but they can be inaccurate for large values of standoff as they are no longer independent of formation properties.

A possible alternative is to introduce inversion-based borehole environmental corrections. Such interpretation methods require developing fast-forward algorithms that accurately simulate borehole environmental effects for borehole nuclear measurements. Rapid numerical simulations based on first-order approximations are inaccurate in the presence of enlarged boreholes because perturbations in the flux sensitivity function give rise to higher-order effects. For neutron measurements, Ijase et al. (2013a) developed the diffusion flux-difference (DFD) method to quantify such flux perturbations in zones with properties that contrast significantly. They showed that sensitivity functions derived with the DFD algorithm yield maximum errors of 1 porosity unit (p.u.) when compared to sensitivity functions calculated in MCNP. However, the DFD algorithm may still yield inaccurate results when the simulated neutron porosity is compared with the neutron porosity estimated from MCNP counts.

For Gamma-Gamma density measurements, Zhou et al. (2009) showed that fast-forward algorithms based on second-order sensitivity functions improve the accuracy of simulated density in the presence of standoff. They yield maximum density errors of 0.02 g/cm^3 at the long-spaced detector and 0.03 g/cm^3 at the short-spaced detector. However, because the MCNP perturbation feature only allows for perturbations in bulk density, cross section, and material composition, second-order sensitivity functions can only be acquired for Gamma-Gamma density measurements. Consequently, second-order fast-forward algorithms cannot be implemented for measurements based on two-particle transport.

To simulate borehole environmental effects in measurements based on two-particle transport, such as spectroscopy and Neutron-Gamma density, it is necessary to quantify sensitivity flux perturbations for neutron-based and photon-based measurements. Therefore, the following advances are required: (1) to improve the accuracy of the DFD algorithm when compared to neutron porosities estimated from MCNP counts, and (2) to derive an alternative method to second-order approximations for the rapid numerical simulation of Gamma-Gamma density measurements; this method should be adaptable to measurements based on two-particle transport.

1.3 RESEARCH OBJECTIVES

The purpose of this dissertation is to explore the limitations and opportunities offered by logging-while-drilling (LWD) Neutron-Gamma density measurements as an alternative to traditional Gamma-Gamma density logging for

in-situ bulk density and porosity estimations. I intend to pursue the following objectives:

- To study the physical processes and nuclear interactions contributing to Neutron-Gamma density measurements. This is achieved by implementing tagging features within MCNP to identify which nuclear interactions contribute to Neutron-Gamma density detector counts and their relative importance for the estimation of bulk density.
- To design a theoretical, albeit realistic, LWD Neutron-Gamma density logging tool using MCNP. Source-detector spacing, choice of detectors, and Monte Carlo modeling assumptions are carefully selected to deliver optimal density accuracy while maintaining realistic physical specifications similar to commercially available logging tools.
- To develop a density estimation algorithm for the interpretation of Neutron-Gamma density detector counts. The algorithm is derived from the fundamental law of gamma-ray attenuation and delivers an accuracy of 0.02 g/cm^3 across complex rock compositions, including various types of shale and anhydrite.
- To compare Neutron-Gamma density and Gamma-Gamma density measurements with respect to properties that are most relevant to petrophysical interpretation practices. The following properties were compared: density accuracy across several types of rock composition, depth of investigation, vertical resolution, measurement response at boundaries between beds exhibiting high density and/or hydrogen index contrasts, and borehole environmental effects.

- To identify the advantages and limitations of Neutron-Gamma density with respect to Gamma-Gamma density measurements. The main advantage of Neutron-Gamma density is the large depth of investigation, which causes the measurement to be less sensitive to the effects of mud-filtrate invasion. A primary limitation includes the lack of density compensation algorithms, such as “spine and rib” methods, necessitating the use of empirical borehole environmental corrections. Limitations also arise for the identification of bed boundaries because Neutron-Gamma density measurements have a lower vertical resolution than Gamma-Gamma density measurements. Further, petrophysical interpretation can also be complicated by asymmetrical log responses at boundaries between layers with sharp contrasts in density and/or hydrogen index.
- To develop a fast-forward numerical algorithm to simulate Neutron-Gamma density measurements in cases where the interpretation provided by the real-time estimation algorithm is inaccurate; for example, when true bulk densities are masked by three-dimensional geometrical and borehole effects. This includes high-angle/horizontal (HA/HZ) wells, thinly-bedded formations, invaded beds, boundaries between beds exhibiting sharp density and/or hydrogen index contrasts, and enlarged boreholes (borehole environmental effects). The fast-forward model is based on first-order perturbation theory and uses precalculated Monte Carlo sensitivity functions. Root-mean-square

errors with respect to MCNP simulations are within 0.023 g/cm^3 for standoff below 1.27 cm (0.5 in).

- To develop higher-order fast modeling methods in order to mitigate borehole environmental effects for neutron and density nuclear measurements. This is the first step in mitigating borehole environmental effects for measurements based on coupled neutron and gamma-ray transport using inversion-based borehole environmental corrections.
 - For neutron measurements, the accuracy of the diffusion flux-difference algorithm introduced by Ijase et al. (2013a) is improved in the presence of standoff by minimizing the size of the borehole perturbations using a two-step fast-forward algorithm.
 - For Gamma-Gamma density measurements, I develop a new fast-numerical-simulation method based on gamma-ray flux-difference approximations. Spatial sensitivity flux perturbations are estimated using gamma-ray point kernel approximations.

1.4 DISSERTATION OUTLINE

To complete the research objectives introduced in the previous section, this dissertation is composed of the present introductory chapter, two technical sections divided into four chapters, and a final chapter containing conclusions and recommendations for future work.

The first technical section of this dissertation, composed of Chapters 2 and 3, provides new measurement and interpretation procedures for Neutron-Gamma

density logging tools. The second technical section of this dissertation is composed of Chapters 4 and 5. Its objective is to develop fast-forward modeling algorithms to simulate and mitigate borehole environmental effects in nuclear measurements.

Chapter 2 introduces an innovative tool design and a density estimation algorithm for Neutron-Gamma density measurements. The Longhorn Neutron-Gamma density tool is designed to capture the variability of the secondary gamma-ray source (in space, energy, and intensity) by introducing two fast neutron detectors. With this new design, the density estimation algorithm is remarkably simple, can be implemented in real time, and delivers density accuracies that compare well to those of Gamma-Gamma density measurements, i.e., 0.012 g/cm^3 in clean formations, and 0.019 g/cm^3 in shales and shaly formations. I also compare Neutron-Gamma density and Gamma-Gamma density measurements with respect to density accuracy, vertical resolution, depth of investigation, and sensitivity to borehole environmental effects.

In Chapter 3, I develop a fast-forward algorithm for simulating Neutron-Gamma density measurements based on first-order approximations. The algorithm can improve petrophysical interpretation of Neutron-Gamma density logs by (1) resolving three-dimensional geometrical effects observed in high-angle/horizontal wells and thinly-bedded formations and (2) mitigating the impact of asymmetrical log responses at bed boundaries exhibiting high density/HI contrasts. However, this algorithm's sensitivity to standoff remains non-negligible because first-order approximations yield density errors greater than 0.03 g/cm^3 for standoff values above 1.27 cm (0.5 in).

Chapter 4 discusses the implementation of a two-step algorithm coupled with diffusion approximations to accurately simulate borehole environmental effects for neutron porosity measurements. The two-step algorithm minimizes the size of the borehole perturbations, thus increasing the validity of the Taylor series approximation. Compared with the neutron porosity derived from MCNP counts, the two-step algorithm yields maximum errors of 2 p.u. in enlarged boreholes.

In Chapter 5, I develop a new method to simulate borehole environmental effects for Gamma-Gamma density measurements. The gamma flux-difference (GFD) method quantifies sensitivity flux perturbations using an exponential point kernel and a Rylov approximation. As opposed to second-order fast-forward algorithms, this method is not limited by the MCNP perturbation feature and can thus be adapted to measurements based on two-particle transport. The method is benchmarked against MCNP and yields density accuracy within 0.03 g/cm³ up to 4.44-cm (1.75-in) standoff.

1.5 LIST OF PUBLICATIONS

Below is a list of journal publications, conference proceedings, and patents related to the research described in this dissertation that were published or will be submitted for review.

1.5.1 Refereed Journal Publications

Luycx M., and C. Torres-Verdín, 2018a, Physics, Applications, and Limitations of Borehole Neutron-Gamma Density Measurements. (*submitted for publication*)

Luycx M., and C. Torres-Verdín, 2018b, Fast modeling of gamma-gamma density measurements via gamma-ray point kernel approximations. (*submitted for publication*)

Luycx M., and C. Torres-Verdín, 2018c, Rapid Forward Modeling of Borehole Logging-While-Drilling Neutron-Gamma Density Measurements. (*to be submitted for publication*)

Ortega E., **M. Luycx**, C. Torres-Verdín, and W. E. Preeg, 2017, Joint petrophysical interpretation of multidetector nuclear measurements in the presence of invasion, shoulder-bed, and well-deviation effects: *Geophysics*, **82**, no. 1, D13–D30.

1.5.2 Refereed Conference Proceedings

Luycx M., and C. Torres-Verdín, 2017, Resolution and accuracy of Neutron-Gamma density measurements compared to conventional Gamma-Gamma density measurements: Paper SPE-187114-MS presented at the SPE Annual Technical Conference and Exhibition, 9-11 October, San Antonio, Texas, USA.

Luycx M., C. Torres-Verdín, O. Mohnke, P. Yuan, F. Inanc, S. Wessling and A. Mezzatesta, 2018, Improvements of Fast Modeling of LWD Neutron Logs Acquired in Enlarged Boreholes with a Commercial Tool: Paper to be presented at the SPWLA Annual Symposium, 2-6 October, London, UK. (*accepted for publication*)

1.5.3 Patents

Miles J., **M. Luycx**, 2017, Measurement of formation bulk density employing forward modeling of neutron-induced gamma-ray emission, U.S. Patent 20,170,160,425; filed December 6, 2015, and issued June 8, 2017. (*issued*)

Guo P., **M. Luycx**, 2016, Method of Rock Mineralogy Interpretation, U.S. Patent filed November 28, 2016. (*filed*)

Chapter 2: Physics, Applications, and Limitations of Borehole Neutron-Gamma Density Measurements

Radioactive chemical sources pose security, health, and environmental risks when employed to estimate rock porosity in-situ. The oil industry has been developing solutions to eliminate radioactive chemical sources in borehole nuclear logging. Pulsed neutron generators have successfully replaced chemical sources in neutron tools, but cesium-137 is still mainly used for borehole density measurements.

Neutron-activated gamma-ray measurements (Neutron-Gamma) are a possible alternative to radioactive chemical sources in density tools. Despite recent advances, the measurement faces challenges regarding density accuracy across diverse solid and fluid rock compositions and non-negligible sensitivity to borehole environmental effects.

I examine a theoretical, albeit realistic Logging-While-Drilling (LWD) Neutron-Gamma density tool operating with two inelastic gamma-ray detectors and two fast neutron detectors. With strong emphasis on measurement physics and source-sensor design, the tool delivers density accuracies comparable to those of Gamma-Gamma density tools with 0.013 g/cm^3 error in shale-free formations, and 0.019 g/cm^3 , in shale and shaly formations. This work also compares Neutron-Gamma density to Gamma-Gamma density in terms of depth of investigation, vertical resolution, and sensitivity to borehole environmental effects to determine optimal logging conditions. Neutron-Gamma density accuracy

is limited in the presence of standoff. With inputs of caliper and mud type, empirical density corrections can be applied up to 0.64-cm (0.25-in) standoff. Neutron-Gamma density also has limited applicability in thinly-bedded formations with maximum vertical resolution of 76 cm (2.5 ft). However, the measurement outperforms Gamma-Gamma density in the presence of invasion because its depth of investigation is twice as large.

2.1 INTRODUCTION

Borehole neutron-porosity tools yield hydrogen content, whereas density tools measure bulk density. These borehole nuclear measurements are key for in-situ porosity estimation and fluid identification. However, rising concerns regarding health, security, and environmental risks call for limiting the use of radioactive chemical sources. Aitken et al. (2002) identified several complicating factors associated with chemical sources: security, storage, transportation, operational safety, and environmental considerations. Chemical sources involve significant precautions for source handling (Kurkoski et al., 1991). They require halting of rig activities for source loading and unloading. They also expose companies to costly retrieval or abandonment measures if the tool is stuck downhole (Rygh and Bonifay, 2000; Gjerdingen et al., 2012). Despite numerous regulations and protocols, sources have been lost or breached (Badruzzaman et al., 2009, Mahiout et al., 2016), sometimes leading to radiation exposure by rig personnel.

Pulsed neutron generators (PNGs) have successfully replaced chemical americium-beryllium (AmBe) neutron sources to perform neutron-based measurements. Because no radioactive particles are emitted when switched-off,

PNGs eliminate many risks, costs, and complications associated with radioactive chemical sources (Gjerdingen et al., 2012).

Thus far, no such practical alternative exists for density tools. Density measurements are primarily acquired with Gamma-Gamma density (GGD) tools that operate radioactive cesium-137 sources. Cesium-137 delivers 662 keV mono-energetic gamma rays at a fixed distance from gamma-ray detectors. At these energy levels and under constant source conditions, gamma-ray attenuation is dominated by Compton scattering and is proportional to electron density. Gamma-Gamma density tools measure density with 0.015 g/cm³ accuracy.

Neutron-Gamma density (NGD) is a sourceless alternative to Gamma-Gamma density. It uses secondary neutron-induced gamma rays to determine bulk density with no chemical source. The concept was originally introduced for density measurements behind casing by Wilson (1995), Odom et al. (1998, 2001), and Neuman et al. (1999). Neutrons emitted with PNGs interact with formation nuclei to generate secondary gamma rays. Compared to Gamma-Gamma density, the measurement presents two complications: First, the secondary gamma-ray source depends on neutron transport and is distributed within the formation in space, energy, and intensity (Inanc, 2014). Coupled with bulk density, formation properties such as hydrogen index impact the tool response. Second, PNGs emit particles at higher energies (14.1 MeV) than cesium-137 (662 keV). Hence, Compton scattering can no longer be considered the dominant interaction.

Early on, Odom et al. (1994, 1997) and Wilson (1995) developed Neutron-Gamma density measurements based on inelastic gamma rays. Inelastic gamma rays are generated through inelastic scattering of fast neutrons and are thus less

affected by porosity variations. Despite these improvements, neutron-activated density measurements remained sensitive to hydrogen index, which led to new designs incorporating neutron detectors to correct for residual source variability. Odom et al. (2001) developed a through-casing sourceless density tool operating with one fast neutron detector. Evans et al. (2012) and Reichel et al. (2012) designed the first commercial radioisotope-free LWD density measurement with thermal and epithermal neutron detectors. They reported accuracies of 0.025 g/cm³ in clean formations and 0.045 g/cm³ in shales. The commercial LWD Neutron-Gamma density tool was compared to Gamma-Gamma density in field studies (Majidi et al., 2012; Atfeh et al., 2013; Alakeely and Meridji, 2014; Kyi et al., 2014; Mahiout et al., 2016) uncovering several limitations, mainly in terms of accuracy (in high-density formations, shales, and shaly formations), and sensitivity to borehole conditions.

Recently, Zhang et al. (2017) introduced a theoretical Neutron-Gamma density logging tool with two gamma-ray detectors measuring inelastic gamma-ray counts and one fast neutron detector. Their interpretation method based on coupled-field theory and Monte-Carlo modeling delivers density estimates within 0.019 g/cm³ accuracy in clean formations with porosity less than 30 porosity units (p.u.) However, Zhang et al. (2017) disregarded the energy dependence of the neutron flux and its effect on inelastic scattering cross sections. It is also difficult to evaluate the quality of the results because the assumptions associated with Monte Carlo modeling of fast neutron and gamma-ray counts were not disclosed by the authors. Moreover, their benchmarking did not include formations with complex mineralogy, such as shales or anhydrite. In the Appendix, I show that

algorithms such as the one derived by Zhang et al. (2017) do not yield accurate density estimates in shale and shaly formations as well as in high-density formations such as anhydrite.

In this chapter, I explore new instrumentation designs and interpretation methods for Neutron-Gamma density. Using MCNP (Monte-Carlo N-particle code, the industry standard for nuclear modeling, Goorley, 2014), I study the measurement physics, and particularly the contribution of each nuclear interaction depending on energy levels. With MCNP, I design a theoretical, but practical, Longhorn Neutron-Gamma density LWD (Logging While Drilling) logging tool that includes two fast neutron detectors and two gamma-ray detectors. Source-detector spacing and estimation algorithm are optimized to secure density accuracies comparable to those of Gamma-Gamma density. Finally, I compare Neutron-Gamma density to Gamma-Gamma density measurements to understand their relative limitations and advantages.

2.2 METHOD

2.2.1 Basic Principles of Gamma-Ray Attenuation and Physics of Gamma-Gamma Density

Gamma-Gamma density is based on gamma-ray attenuation through Compton scattering interactions. Gamma rays of energy 662 KeV are emitted by radioactive cesium-137 at a constant rate and at a fixed distance from the detectors. The fundamental law of gamma-ray attenuation (Lamarsh and Baratta, 2001) states that

$$\psi_{GR} = \psi_i \cdot \exp(-\mu_{m-To} \cdot \rho_b \cdot \ell) , \quad (2.1)$$

where ψ_{GR} is gamma-ray flux exiting the material, ψ_i is initial flux, ℓ is thickness of the attenuating medium, μ_{m-To} is total mass attenuation coefficient, and ρ_b is material bulk density. The total mass attenuation coefficient μ_{m-To} is decomposed as

$$\mu_{m-To} = \mu_{m-Co} + \mu_{m-Pa} + \mu_{m-Ph} , \quad (2.2)$$

where μ_{m-Co} is Compton mass attenuation coefficient per atom, μ_{m-Pa} and μ_{m-Ph} are pair production and photoelectric mass attenuation coefficients, respectively. Mass attenuation coefficients in equation 2.2 are plotted in **Figure 2.1** as a function of gamma-ray energy for common lithologies. Compton scattering is the dominant interaction between 140 and 662 keV, the energy range of Gamma-Gamma density measurements (**Figure 2.1b**). For Gamma-Gamma density, the total mass attenuation coefficient, μ_{m-To} , thus approximately equals the Compton mass attenuation coefficient per atom, μ_{m-Co} , i.e.,

$$\mu_{m-To} \approx \mu_{m-Co} . \quad (2.3)$$

The Compton mass attenuation coefficient per atom, μ_{m-Co} , is defined as

$$\mu_{m-Co} = \frac{Z}{A} N_{Av} \cdot \sigma_{Co} , \quad (2.4)$$

where Z is atomic number, A is atomic mass, N_{Av} is Avogadro's number, and σ_{Co} is Compton scattering microscopic cross section per electron. Gamma-ray flux measured at the Gamma-Gamma density detectors, ψ_{GGD} , is thus expressed as

$$\psi_{GGD} \approx \psi_i \cdot \exp\left(-N_{Av} \cdot \sigma_{Co} \cdot \frac{\rho_e}{2} \cdot \ell\right), \quad (2.5)$$

where electron density, ρ_e , is defined as

$$\rho_e = 2 \frac{Z}{A} \rho_b. \quad (2.6)$$

In Gamma-Gamma density, the use of a chemical source ensures that the initial gamma-ray flux, ψ_i , and the source-detector distance, ℓ , are constant in equation 2.5. It follows that the logarithm of gamma-ray counts varies linearly with electron density and that bulk density can be estimated by monitoring gamma-ray count rates. Throughout this chapter, the above behavior is referred to as the linear attenuation of gamma rays with density.

2.2.2 Physics and Principles of Neutron-Gamma Density

Neutron-Gamma density tools make use of pulsed neutron sources to generate high-energy 14.1 MeV fast neutrons that excite formation nuclei. Neutron-Gamma density uses gamma rays generated upon de-excitation to estimate density.

At energy levels below 14.1 MeV, neutrons produce gamma rays via three interactions. On one hand, high-energy neutrons generate gamma rays through

inelastic scattering, or, through (n,x) interactions. In the latter reaction, n represents neutron, and x represents any particle such as neutron, n , proton, p , deuteron, d , alpha, α , or a combination of all of them; (n,x) interactions include, for instance, $(n,2n)$, (n, α) , $(n,n' \alpha)$, (n,p) or (n,d) interactions. These are threshold reactions: neutrons require a minimum excitation energy. In common lithologies, the threshold is around 1 MeV for inelastic scattering, and around 4 MeV for (n,x) interactions. On the other hand, lower energy (mostly thermalized) neutrons can undergo radiative capture upon interacting with a nucleus. The nucleus emits capture gamma rays when decaying back to its ground state. Capture gamma-ray emission is highly dependent on hydrogen index because neutron transport is dominated by diffusion at thermal energy levels. To minimize the influence of hydrogen index, Neutron-Gamma density is thus based on non-capture gamma-ray counts, following the approach introduced by Odom et al. (1994, 1997) and Wilson (1995). Non-capture gamma rays include not only inelastic gamma rays but also gamma rays emitted through (n,x) interactions, and by annihilation and bremsstrahlung radiations.

Annihilation gamma rays are produced following a gamma reaction called pair production. A gamma-ray photon of energy in excess of 1.02 MeV can interact with a nucleus. The photon disappears and a positron-electron pair is formed, while the electron and positron usually neutralize one another and produce annihilation radiation consisting of two 0.51-MeV photons. Pair production has a lower energy threshold of 1.02 MeV and becomes non-negligible at energies above ~9 MeV in common lithologies (**Figure 2.2.1b**). Free electrons are generated through Compton scattering and pair production interactions. When approaching a

nucleus, they can undergo sudden deceleration and deflection, leading to bremsstrahlung gamma-ray emission. **Figure 2.2** describes and summarizes all nuclear interactions contributing to Neutron-Gamma density.

In MCNP, I model non-capture gamma-ray counts by introducing a neutron energy cutoff at 1 MeV. Any neutron whose energy falls below that threshold is killed, effectively limiting the probability of radiative capture. Using MCNP tagging features, the contribution of each reaction to non-capture gamma-ray counts is examined in **Figure 2.3**. Panel (a) analyses the distribution of nuclear interactions considering the last production event before Compton scattering, while panel (b) considers the last collision event. Annihilation gamma rays represent the main contribution to Neutron-Gamma density in terms of gamma-ray production events (56%). Inelastic scattering and (n,x) interactions also produce significant contributions, 21%, and 15%, respectively. **Figure 2.3a** establishes that the non-linear attenuation of total gamma-ray counts stems from inelastic gamma rays. This behavior is explained by studying the influence of hydrogen index on fast neutrons depending on energy levels. In **Figures 2.4 and 2.5**, I model fast neutron flux within freshwater-filled limestone formations between 1 and 4 MeV, and above 4 MeV. Neutron flux is unaffected by porosity above 4 MeV. However, between 1 and 4 MeV, total flux (**Figure 2.4**) and the spatial extension of the neutron cloud (**Figure 2.5a**) are both influenced by hydrogen index. The fast neutron cloud is on average 13 cm (5 in) closer to the tool boundary when porosity increases by 30 p.u. Therefore, gamma rays generated through inelastic scattering (between 1 and 14.1 MeV) are relatively more affected by hydrogen index variations than gamma

rays generated through annihilation or (n,x) interactions, whose energy thresholds are both located above 4 MeV.

Even though pair production contributes to 56% of total gamma-ray counts (considering the last production event), Compton scattering is the last collision event for 86% of gamma rays arriving at the detector in freshwater-filled limestone (**Figure 2.3b**). Most gamma rays are Compton scattered after pair production and annihilation events. Overall, non-capture gamma-ray counts obey the gamma-ray attenuation behavior described in equation 2.1.

2.2.3 Neutron-Gamma Density Tool Design

I introduce a new theoretical, albeit practical Logging-While-Drilling (LWD) Neutron-Gamma density tool designed and tested via MCNP modeling. The Longhorn Neutron-Gamma density tool is optimized to minimize the impact of fast neutron transport on gamma-ray counts. To that end, it includes four detectors: two cerium-doped lanthanum bromide $[\text{LaBr}_3(\text{Ce})]$ gamma-ray detectors, and two fast neutron detectors. It also operates a pulsed neutron source that generates 14.1 MeV fast neutrons during burst intervals of 10 microseconds. **Figure 2.6** describes the fast neutron flux inside a 0 p.u. limestone block with respect to neutron energy at different times during and after the burst. After the burst, the energy of neutrons immediately falls below the inelastic scattering energy threshold of 1 MeV. Therefore, gamma rays are only measured during the 10-microsecond interval of the burst to minimize contributions from capture gamma rays.

To secure density accuracies comparable to Gamma-Gamma density measurements, the gamma-ray long-spaced detector (GRLS) is located 90 cm (35

in) from the source. At this distance, the slope of gamma-ray count attenuation with density is similar to that achieved halfway between the short- (SSn) and long-spaced (LSn) gamma-ray detectors in a Gamma-Gamma density tool (**Figure 2.7**). Increasing source-detector spacing beyond 90 cm (35 in) is detrimental to counts statistics with little gain in accuracy. The short-spaced gamma-ray detector (GRLS) is located 50 cm (20 in) from the source. Fast neutron detectors are used to capture the variations of the secondary gamma-ray source in space and intensity. Hence, they are located in front of each gamma-ray detector, at 35 and 75 cm (14 and 30 in) from the source, respectively. **Figure 2.8** describes the Longhorn Neutron-Gamma density tool design, and **Table 2.1** summarizes the corresponding geometrical properties.

2.2.4 Neutron-Gamma Density Detector Modeling with MCNP

The density accuracy of Neutron-Gamma density tools is highly sensitive to gamma-ray and fast neutron counts. Therefore, modeling assumptions made when simulating gamma-ray and fast neutron counts in MCNP are compared to acquisition procedures and detector designs used for commercial logging tools.

The net inelastic gamma spectrum measured in the borehole with commercial logging tools is obtained by removing the contribution of the early capture spectrum (acquired after the 10 microseconds burst) to the burst spectrum, using a subtraction factor (Radtke et al., 2012). This subtraction factor varies depending on the macroscopic thermal neutron capture cross section (Inanc, 2014). Inelastic gamma-ray counts are then determined by integrating the net inelastic gamma-ray spectrum over all energy bins. Because of constraints associated with pulse-height spectra modeling in MCNP, the Longhorn Neutron-

Gamma density tool estimates non-capture gamma-ray counts with a simplified procedure that invokes a neutron energy cutoff at 1 MeV. It follows that this design does not consider the impact of the macroscopic thermal neutron capture cross section on inelastic gamma-ray counts. The tool operates lanthanum bromide [LaBr₃(Ce)] scintillators, but sodium iodide (NaI) detectors would also be acceptable: because gamma-ray counts are summed over all energy bins, light output and efficiency are more critical than energy resolution.

Existing commercial Neutron-Gamma density logging tools attempt to reproduce fast neutron counts using epithermal and thermal neutron detectors (Reichel et al., 2012, Evans et al., 2012). Diamond fast neutron detectors prepared via chemical vapor deposition were developed for source monitoring in high-temperature, high-shock logging environments (Philip et al., 2017). With intrinsic diamond layer thickness of 53 μm , they provide a counting efficiency of 0.78% for 14.8 MeV neutrons (Almaviva et al., 2008). However, they have only recently been introduced in logging tools, and exclusively for source monitoring (Rose et al., 2015). Plastic scintillators sustaining high operating temperatures were also patented to detect fast neutrons in well-logging applications (Hall, 1964; Odom et al., 2001, 2002; Simonetti et al., 2005). Simonetti et al. (2005) introduced a plastic scintillator that selectively detects fast neutrons above 0.5 MeV while retaining good mechanical properties in high-temperature environments. Odom et al. (2001, 2002) developed a fast neutron detector with alternating layers of activated zinc sulfide scintillator (ZnS) and transparent plastic, providing counting efficiency of 3.8% for 4.1 MeV neutrons (Emmerich, 1954). Fast neutrons interact with the plastic material and generate recoil protons. Then, scintillation photons are

generated within ZnS by the incident protons. They can escape ZnS through the transparent plastic material and are detected by the photomultiplier tube. Due to the complexity of the reactions involved in consecutive materials, modeling a ZnS detector in MCNP would call for experimental benchmarking. Therefore, this new design alternatively includes helium-4 scintillation detectors pressurized at 20 bar (Chandra et al., 2012). Such detectors can be used to detect fast neutrons because the elastic cross section of helium-4 is relatively larger in the energy range above 0.5 MeV. Their counting efficiency (0.035% for 4 MeV neutrons) is lower than that of ZnS scintillators because helium-4 has low density. However, they can be realistically modeled in MCNP by multiplying the neutron flux inside the detector by the elastic scattering cross section of helium-4. Additionally, the fast neutron detector design includes a 1 MeV lower energy bin. In the section on density accuracy below, I show that this energy bin can be lowered to 0.01 MeV without decreasing accuracy: the Longhorn tool design allows significant flexibility in terms of energy range at fast neutron detectors. **Figure 2.9** displays the inputs of the four detectors with respect to density for common rock compositions. Helium-4 fast neutron detectors tally fast neutrons detected above 1 MeV, while gamma-ray counts are obtained with a 1 MeV neutron energy cutoff.

2.2.5 Density Estimation Algorithm

Pair production and Compton scattering both contribute significantly to total detectors counts, with pair production representing 56% of gamma-ray counts considering the last production event, and Compton scattering, 86%, considering the last collision event. The exiting gamma-ray flux in equation 2.1 can be rewritten as

$$\psi_{GR} = \psi_i \cdot \exp[-(\mu_{m-Co} + \mu_{m-Pa}) \cdot \rho_b \cdot \ell], \quad (2.7)$$

with

$$\mu_{m-To} \approx \mu_{m-Co} + \mu_{m-Pa} \quad (2.8)$$

The total mass attenuation coefficient, μ_{m-To} , is approximately constant with lithology between 1 and 14.1 MeV (**Figure 2.1a**). If I approximate the gamma-ray flux at each detector, ψ_{GR} , by gamma-ray counts, and the initial gamma flux, ψ_i , by fast neutron counts (the source of the secondary gamma rays), one can write

$$GRLS \approx FastF \cdot \exp(-\mu_{m-To} \cdot \rho_b \cdot \ell_{LS}), \quad (2.9)$$

and

$$GRSS \approx FastN \cdot \exp(-\mu_{m-To} \cdot \rho_b \cdot \ell_{SS}), \quad (2.10)$$

where ℓ_{LS} designates the distance between the site of gamma-ray generation and the long-spaced gamma-ray detector, and ℓ_{SS} is the distance between the site of gamma-ray origination and the short-spaced gamma-ray detector; $GRLS$ designates non-capture gamma-ray counts at the long-spaced gamma detector, and $GRSS$, at the short-spaced gamma detector; $FastF$ designates neutron counts at the far fast neutron detector, and $FastN$ at the near fast neutron detector.

The distances ℓ_{LS} and ℓ_{SS} vary with the location of gamma-ray generation and change depending on formation composition. However, $L = \ell_{LS} - \ell_{SS}$ should remain relatively constant as ℓ_{LS} and ℓ_{SS} are similarly affected by changes in rock composition. Therefore, dividing equation 2.9 by equation 2.10, one obtains

$$\begin{aligned} \frac{GRLS}{GRSS} &\approx \frac{FastF}{FastN} \cdot \exp[-\mu_{m-To} \cdot \rho_b \cdot (\ell_{LS} - \ell_{SS})] \\ &\approx \frac{FastF}{FastN} \cdot \exp(-\mu_{m-To} \cdot \rho_b \cdot L) \end{aligned} \quad (2.11)$$

Equation 2.11 can be rewritten as

$$\log_e \left(\frac{GRLS}{GRSS} \right) - \log_e \left(\frac{FastF}{FastN} \right) \approx -\mu_{m-To} \cdot L \cdot \rho_b, \quad (2.12)$$

where $-\mu_{m-To} \cdot L$ remains relatively constant when rock composition changes. By trial and error, I found that the following expression improves the overall accuracy:

$$Corrected \text{ gamma ray counts} = \log_e \left(\frac{GRLS}{GRSS} \right) - \sum_{i=0}^2 a_i \log_e \left(\frac{FastF}{FastN} \right)^i = m_1 \cdot \rho_b. \quad (2.13)$$

The unknowns a_i represent the fitting coefficients of a polynomial expression whose variable is the logarithm of the ratio of fast neutron counts. Similarly, m_1 is a fitting coefficient whose value is closely related to the constant $-\mu_{m-To} \cdot L$. Fitting coefficients a_i and m_1 are obtained by solving the linear inverse problem $\mathbf{Ay}=\mathbf{b}$ using a least square minimization algorithm (Aster et al., 2005), with

$$\mathbf{A} = \begin{bmatrix} 1 & \log_e \left(\frac{FastF_1}{FastN_1} \right) & \log_e \left(\frac{FastF_1}{FastN_1} \right)^2 & \rho_{b,1} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \log_e \left(\frac{FastF_k}{FastN_k} \right) & \log_e \left(\frac{FastF_k}{FastN_k} \right)^2 & \rho_{b,k} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \log_e \left(\frac{FastF_{ktot}}{FastN_{ktot}} \right) & \log_e \left(\frac{FastF_{ktot}}{FastN_{ktot}} \right)^2 & \rho_{b,ktot} \end{bmatrix}, \quad (2.14)$$

$$\mathbf{y} = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ m_1 \end{bmatrix}, \quad (2.15)$$

and

$$\mathbf{b} = \begin{bmatrix} \log_e \left(\frac{GRLS_1}{GRSS_1} \right) \\ \vdots \\ \log_e \left(\frac{GRLS_k}{GRSS_k} \right) \\ \vdots \\ \log_e \left(\frac{GRLS_{ktot}}{GRSS_{ktot}} \right) \end{bmatrix}, \quad (2.16)$$

where gamma-ray and neutron counts are computed in *ktot* formations of different bulk densities, $\rho_{b,k}$. **Table 2.2** displays the coefficients a_i and m_1 for the Longhorn Neutron-Gamma density tool. Results of the density estimation algorithm are presented in **Figure 2.10** for a wide range of commonly encountered rock

compositions. The estimation algorithm, which is based on the fundamental law of gamma-ray attenuation, remains valid when the linear inverse problem, $\mathbf{Ay}=\mathbf{b}$, is solved using limited input data (**Figure 2.11**), indicating that it accurately captures the physics of the measurement.

2.3 RESULTS: COMPARISON BETWEEN NEUTRON-GAMMA DENSITY AND GAMMA-GAMMA DENSITY

I compare the properties of Neutron-Gamma density and Gamma-Gamma density measurements. **Table 2.1** describes the geometrical properties of the Gamma-Gamma density tool used in the comparison. Its long-spaced and short-spaced gamma-ray detectors are located 41.9 cm and 21.6 cm (16.5 in and 8.5 in) from the source, respectively (Ijasan et al., 2011).

2.3.1 Density Accuracy

High density accuracy is the main focus of the Longhorn Neutron-Gamma density tool design to ensure reliable porosity estimates in formations with complex mineralogy. **Figure 2.12** examines the accuracy of the density estimation algorithm for different types of rock compositions, such as clean formations filled with freshwater, brine, oil, and gas, shales and shaly formations, and anhydrite. I compare Neutron-Gamma density accuracies considering different energy ranges at the fast neutron detectors. The estimation algorithm yields similar accuracies for the energy ranges 0.01 to 14.1 MeV, 0.1 to 14.1 MeV, 0.5 to 14.1 MeV, and 1 to 14.1 MeV.

Using fast neutrons counts in the energy range between 1 and 14.1 MeV, the estimation algorithm yields accuracies of 0.012 g/cm³ in clean formations, and

0.019 g/cm³ in shale and shaly formations (**Figure 2.13a**). The overall accuracy is 0.0148 g/cm³ (**Figure 2.13b**). Measurement accuracy compares well to that of Gamma-Gamma density (0.015 g/cm³ at the short-spaced detector). It is improved by more than 100% when compared to the accuracies of 0.025 g/cm³ in clean formations and 0.045 g/cm³ in shale and shaly formations reported by Reichel et al. (2012) and Evans et al. (2012). Furthermore, the Longhorn tool remains accurate in high-density formations such as anhydrite (**Figure 2.13a**).

The Longhorn Neutron-Gamma density tool secures density accuracies comparable to those achieved by Gamma-Gamma density measurements. However, the tools are affected differently by borehole environmental effects because Neutron-Gamma density is more sensitive to standoff in enlarged boreholes. Neutron-Gamma density also exhibits increased depth of investigation, and consequently, lower vertical resolution.

2.3.2 Depth of Investigation

There is no convention for defining depth of investigation. A common definition quantifies the depth of investigation as the radius corresponding to 90% of the radial geometrical function (Ellis and Singer, 2007). This definition is too optimistic when determining the effective radial distances over which a measurement is sensitive (Moake, 2014). Yet, this value is often advertised by vendors and can be used as a means of comparison between Neutron-Gamma density and Gamma-Gamma density.

The radial geometrical function is obtained by integrating flux sensitivity functions (FSFs) in the radial direction. Flux sensitivity functions account for the geometrical importance of the formation. Thus, they quantify perturbed detector

counts using linear perturbations in formation cross sections. The concept of flux sensitivity function was first introduced by Watson (1984, 1992) and Case et al. (1994). I use the method developed by Mendoza et al. (2010a) to generate flux sensitivity functions for the Longhorn Neutron-Gamma density, and Gamma-Gamma density tools. **Figure 2.14** compares the radial geometrical functions of Neutron-Gamma density and Gamma-Gamma density for different porosities, formation fluids, and lithologies. The depth of investigation of Neutron-Gamma density is approximately 24 cm (9.5 in). It is twice as large when compared to that of Gamma-Gamma density. Moreover, it remains unaffected by formation properties, in particular, by porosity (**Figure 2.14a**).

Alternatively, the radial geometrical function can be calculated when water invades a gas-filled formation (Moake, 2014). In **Figure 2.15**, I study the piston-like invasion of 25 kppm NaCl water-base mud into a 30 p.u. gas-filled limestone formation. At 90% of the measurement response between invaded (2.202 g/cm^3) and virgin (1.927 g/cm^3) bulk densities, i.e., at 2.174 g/cm^3 , the depth of investigation is approximately 25 cm (10 in) for Neutron-Gamma density and 11 cm (4.3 in) for Gamma-Gamma density at the long-spaced detector. Owing to its relatively large depth of investigation, Neutron-Gamma density is less affected by the presence of invasion. With no invasion, the uncertainty in the relationship between electron and bulk density (equation 2.6) causes relatively lower density accuracy for the Gamma-Gamma density measurement.

2.2.4 Vertical Resolution

The larger depth of investigation of Neutron-Gamma density comes with a compromise against decreased vertical resolution. I study the vertical resolution

with perturbations introduced by a 20 p.u. freshwater-filled limestone formation (2.368 g/cm^3) (**Figure 2.16a**), and a 25 p.u. gas-filled limestone formation (2.0825 g/cm^3) (**Figure 2.16b**), to a 0 p.u. limestone background medium (2.71 g/cm^3). The vertical resolution of Neutron-Gamma density is estimated at 76 cm (2.5 ft), whereas Gamma-Gamma density has a resolution of at least 60 cm (2 ft) at the long-spaced detector and 30 cm (1 ft) at the short-spaced detector. In **Figure 2.16**, Neutron-Gamma density also exhibits an asymmetric response at boundaries between beds exhibiting large contrasts in density or hydrogen index.

2.3.5 Borehole Environmental Effects

In Gamma-Gamma density logs, borehole environmental effects are compensated for using methods derived from the “spine and rib” technique (Wahl et al., 1964). This technique takes advantage of the dual measurement performed at long- and short-spaced detectors and does not require inputs of borehole size, standoff, or mud type.

Neutron-Gamma density requires inputs from four detectors to produce one density measurement. As explained using the fundamental law of gamma-ray attenuation, these inputs are necessary to correct for the variability of the secondary gamma-ray source. Such a requirement prevents one from using the spine-and-rib technique for Neutron-Gamma density. Inputs for standoff, borehole size, and mud type are required to perform borehole environmental corrections.

Neutron-Gamma density is particularly sensitive to standoff, especially in conjunction with light mud where the measured density is shifted closer to mud density. **Figures 2.17** and **2.18** show density corrections with increasing standoff depending on mud type, lithology, and porosity. When standoff remains below 0.64

cm (0.25 in), the correction on density is independent of changes in formation lithology or porosity, and the inputs for density correction can be limited to caliper and mud type. The impact of increasing borehole size on Neutron-Gamma density measurements is highly correlated to standoff value. A larger borehole will have minimum effect on the measurement at the bottom sector if the tool is eccentric (standoff is zero). However, density corrections are required if the tool is centered, or if density is measured in different azimuthal sectors (**Figure 2.19**).

2.4 DISCUSSION

This work aims to develop a sourceless density measurement with accuracies similar to those of Gamma-Gamma density tools, including in complex mineralogy. To that end, the Longhorn Neutron-Gamma density tool design includes two helium-4 fast neutron detectors. Fast neutron scintillators with higher efficiency such as ZnS-based scintillators have been patented for use in downhole environments, but they have yet to be incorporated in commercial logging tools. To this date, commercial Neutron-Gamma density tools use epithermal and thermal neutron detectors to emulate fast neutron counts. I believe that Neutron-Gamma density tools require at least two fast neutron detectors to match the accuracy of Gamma-Gamma density tools. Previous attempts at emulating fast neutron counts using lower-energy neutrons increased density errors by more than 100% when compared to Gamma-Gamma density (Reichel et al., 2012, Evans et al., 2012). Similarly, designs featuring a single fast neutron detector cannot adequately capture source variability in complex mineralogy. Zhang et al. (2017) introduced a theoretical Neutron-Gamma density tool with two gamma-ray

detectors and one fast neutron detector. They developed a density estimation algorithm and reported maximum density errors of 0.019 g/cm^3 in clean formations up to 30 p.u. However, the algorithm was not benchmarked across complex mineralogy, such as shales or anhydrite. In the Appendix, I implement linear inversion to determine the unknown parameters in the density algorithm of Zhang et al. (**Table A.1**). For the Longhorn Neutron-Gamma density tool, the density algorithm developed by Zhang et al. delivers root-mean-square density errors of 0.015 g/cm^3 in clean formations. In shales and anhydrite, root-mean-square errors are 0.05 g/cm^3 and 0.1 g/cm^3 , respectively (**Figure A.2**). In complex mineralogy, density errors therefore increase by more than 150% when compared to those achieved with the Longhorn density estimation algorithm (**Figure 2.12**).

There is an opportunity for extracting information from gamma rays produced by neutrons whose energy exceeds 4 MeV. I established that high-energy neutrons (above 4 MeV) are almost unaffected by changes in hydrogen index: the neutron-induced secondary gamma-ray source remains virtually constant when porosity changes. Above 4 MeV, the fast neutron flux remains at the same radial distance when porosity increases by 60 p.u (**Figure 2.5**). By designing appropriate pulsing-schemes to allow for sufficient count statistics, density could be measured from secondary gamma rays induced by high-energy neutrons (above 4 MeV). In **Figure 2.20**, I study the attenuation of non-capture gamma rays detected above (panel a) and below (panel b) 4 MeV. Above 4 MeV, gamma-ray counts measured at the long-spaced gamma-ray detector decrease by an order of magnitude when compared to gamma-rays measured between 0.1 and

14.1 MeV. However, examination of inelastic gamma-ray counts above 4 MeV in panel (b) shows that gamma-ray attenuation is independent of porosity.

Finally, one of the main limitations of Neutron-Gamma density is its susceptibility to borehole environmental effects, mainly standoff. There are two possibilities for mitigating this problem. One possibility is to design a Neutron-Gamma density tool with an additional gamma-ray detector to allow for the implementation of the spine-and-rib technique. A second possibility is to take advantage of interpretation methods based on fast modeling and inversion to simulate and correct for borehole environmental effects in real time. Fast modeling techniques were used successfully to estimate properties such as radius of investigation in Sigma measurements (Ortega et al., 2017). Standoff can be similarly interpreted in the form of a contrast in properties along the radial direction. Fast-forward modeling can facilitate well log interpretation in cases where standoff is too large (greater than 0.64 cm or 0.25 in) for density corrections based on empirical relationships. At boundaries between beds exhibiting large contrasts in density or hydrogen index resulting in asymmetrical log behavior, fast modeling techniques can also improve the results of the density estimation algorithm.

2.5 CONCLUSIONS

Neutron-Gamma density measurements are based on complex nuclear interactions whose relative contributions vary with particle energy levels and rock composition. I developed a new approach for the interpretation of Neutron-Gamma density measurements using an innovative tool design. Two helium-4 fast neutron detectors evaluate the spatial distribution and intensity of the secondary gamma-

ray source. They correct non-capture gamma-ray counts for source variability according to the fundamental law of gamma-ray attenuation. Consequently, the proposed new density estimation algorithm does not require corrections based on information from other well logs and can be executed in real time while drilling. Its associated fitting coefficients can also be adapted for measurements behind casing.

With this new design and interpretation method, the average accuracy of Neutron-Gamma density (0.0148 g/cm^3) compares well to that of Gamma-Gamma density. Such accuracy is maintained across a wide range of rock compositions, independently of mineralogy, formation bulk density, formation fluid, or fluid salinity. Particularly, the measurement delivers accurate density estimates in shale and shaly formations (0.019 g/cm^3 accuracy), in gas-filled formations, and in high-density formations such as anhydrite. Compared to Gamma-Gamma density, Neutron-Gamma density tools have relatively low vertical resolution (76 cm or 2.5 ft), which causes non-negligible spatial averaging effects across thinly bedded formations, but their depth of investigation is twice as large.

A detailed comparison against Gamma-Gamma density uncovers several practical limitations: Neutron-Gamma density tools perform poorly in the presence of large standoff, which should be kept under 0.64 cm (0.25 in). Other well logs should be used to identify bed boundaries because Neutron-Gamma density exhibits relatively low vertical resolution and delivers asymmetrical log responses at boundaries between beds exhibiting large contrasts in hydrogen index or density. Presence of nonlinear asymmetrical effects can also complicate petrophysical interpretations. Nonetheless, forward modeling and inversion have

successfully been used with other nuclear tools to improve log interpretation in complex formations and well geometries. These techniques could be implemented with Neutron-Gamma density to correct for standoff effects and asymmetrical tool responses in real time.

Variable	Longhorn Gamma-Gamma density tool [cm]	Longhorn Neutron-Gamma density tool [cm]
Tool diameter	10.795	10.16
GRLS detector distance	41.9	90
GRLS detector diameter	2.3	5
GRLS detector length	5	9
GRSS detector distance	21.6	50
GRSS detector diameter	2.3	5
GRSS detector length	5	9
Far Fast Neutron detector distance	/	75
Far Fast Neutron detector diameter	/	5
Far Fast Neutron detector length	/	8
Near Fast Neutron detector distance	/	35
Near Fast Neutron detector diameter	/	5
Near Fast Neutron detector length	/	8

Table 2.1. Geometrical properties of the Longhorn Gamma-Gamma density and Neutron-Gamma density tools. Detector distances are measured from the source location.

Fitting coefficient	Value
a_0	14.8880
a_1	- 20.4645
a_2	6.0101
m_1	- 0.8035

Table 2.2. Coefficients used in the density estimation algorithm.

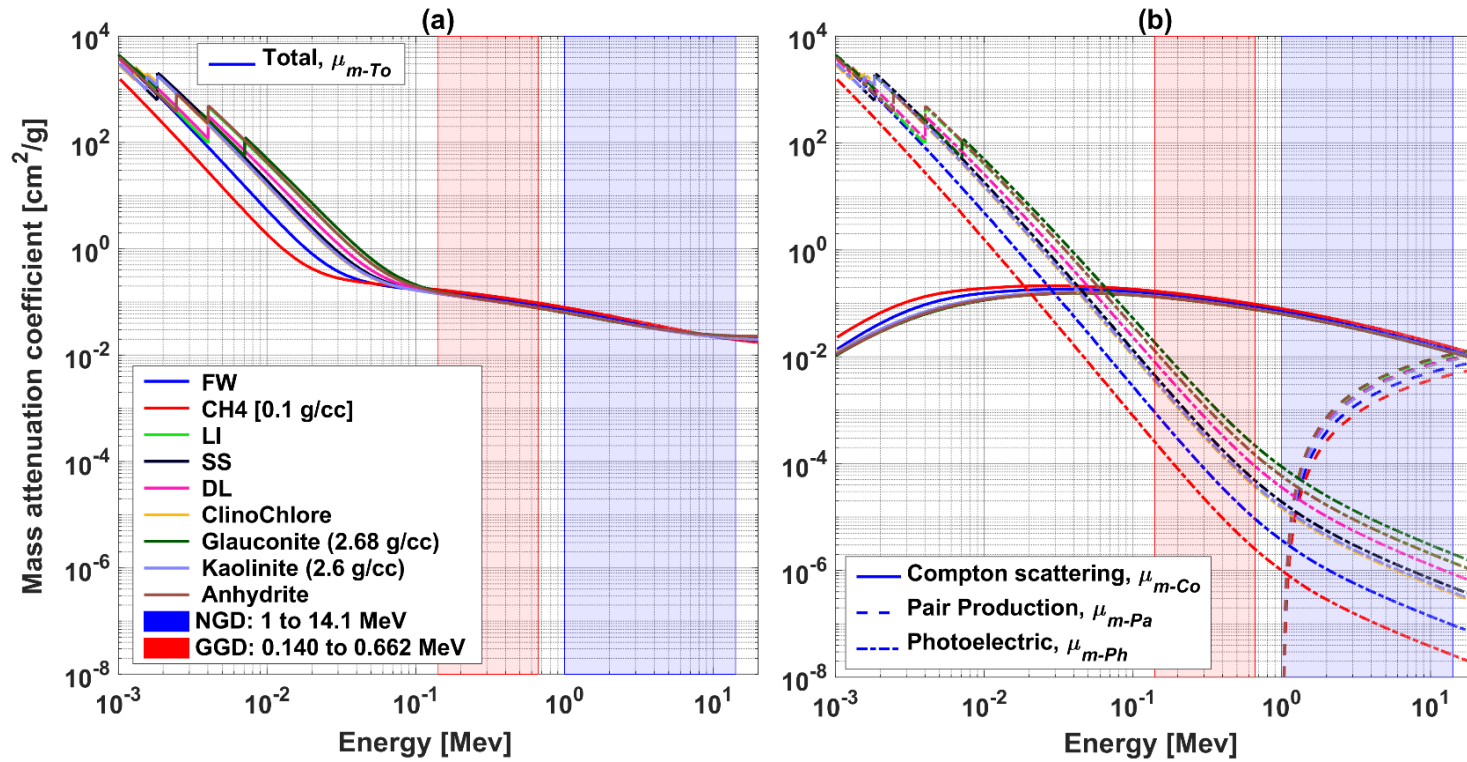


Figure 2.1. (a) Total mass attenuation coefficient and (b) mass attenuation coefficient for Compton scattering, pair production and photoelectric interactions as a function of gamma-ray energy for fresh water, methane, clean formations, shales, and anhydrite. The energy range of Gamma-Gamma density measurements (between 140 and 662 keV), and Neutron-Gamma density measurements (between 1 and 14.1 MeV) are identified by red and blue areas, respectively. FW stands for freshwater, CH4, for methane, LI, for limestone, SS, for sandstone, and DL, for dolomite.

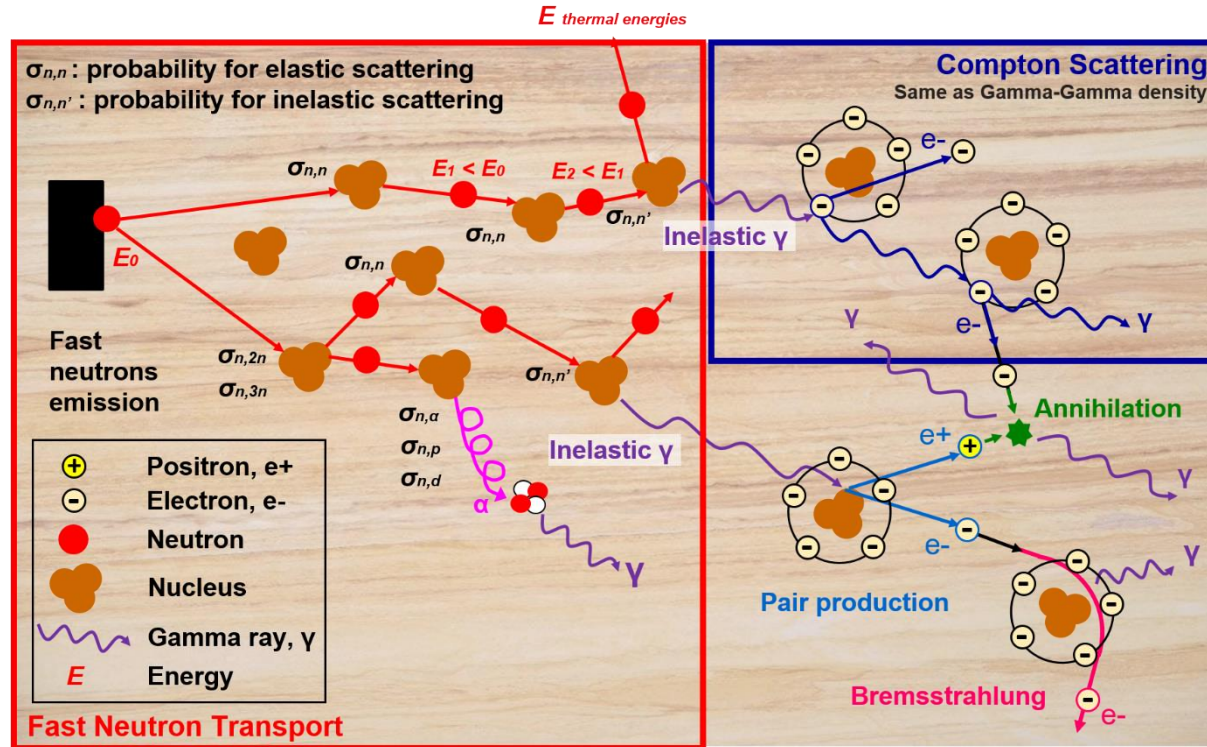


Figure 2.2. Description of the nuclear interactions contributing to Neutron-Gamma density measurements, including fast neutron transport and gamma-ray transport. Secondary gamma rays are emitted during fast neutron transport through inelastic scattering or (n,x) interactions, where (n,x) interactions include, for example, $(n,2n)$, (n,α) , $(n,n'\alpha)$, (n,p) , $(n,n'p)$ or (n,d) interactions. During gamma-ray transport, secondary gamma rays are generated through Compton scattering, pair production, annihilation, and bremsstrahlung interactions.

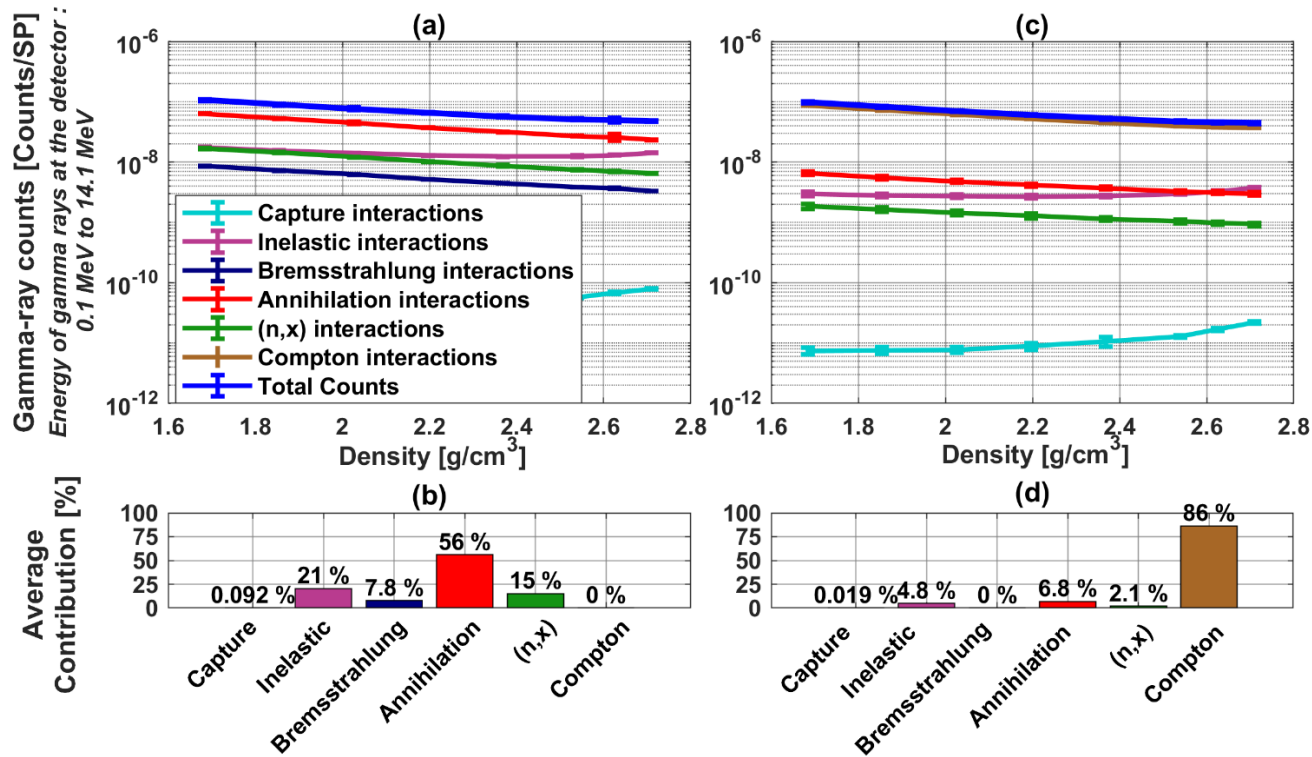


Figure 2.3. (a) Analysis of nuclear interactions contributing to total Neutron-Gamma density gamma-ray counts considering the last production event (subsequent Compton scattering events are ignored), and (b) equivalent average contributions in percentage of total counts; (c) similar to (a) considering the last collision interaction, with (d) equivalent average contributions in percentage of total counts, for a freshwater-filled limestone formation. (n,x) interactions include, for example, (n,2n), (n, α), (n,n' α), (n,p), (n,n'p) or (n,d) interactions.

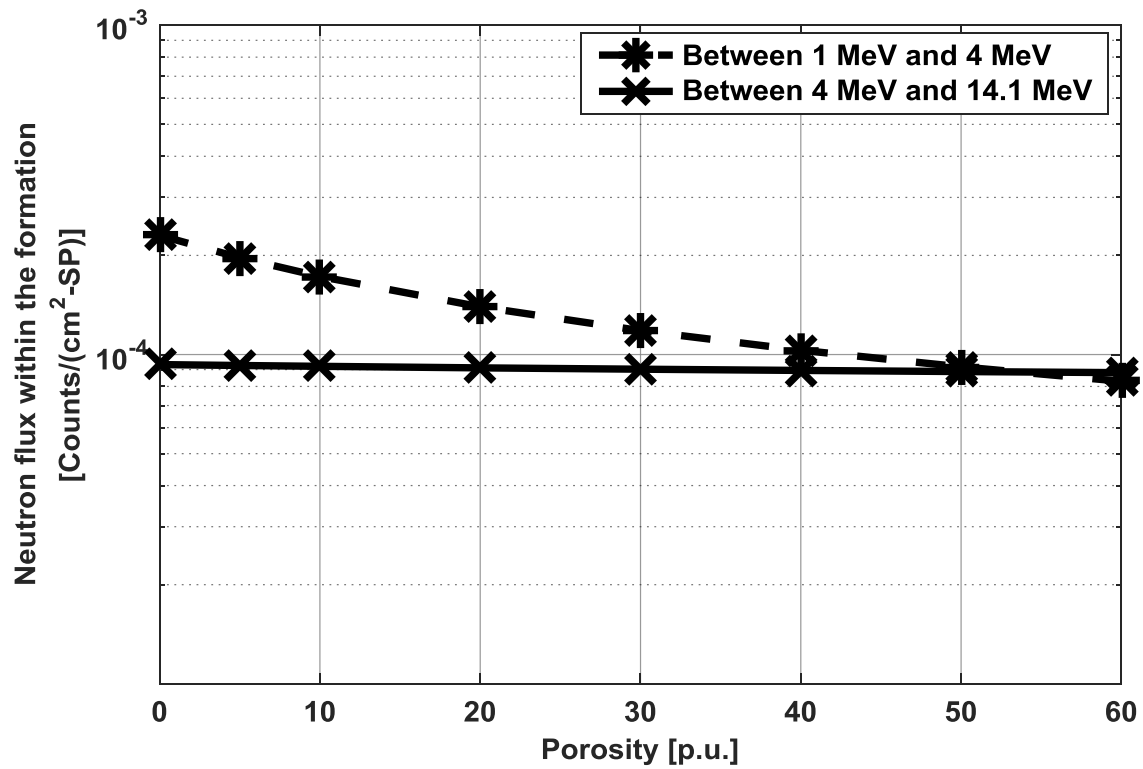


Figure 2.4. Neutron flux within freshwater-filled limestone formations depending on porosity (hydrogen index) for neutrons with energies between 1 and 4 MeV (solid line), and between 4 and 14.1 MeV (dashed line).

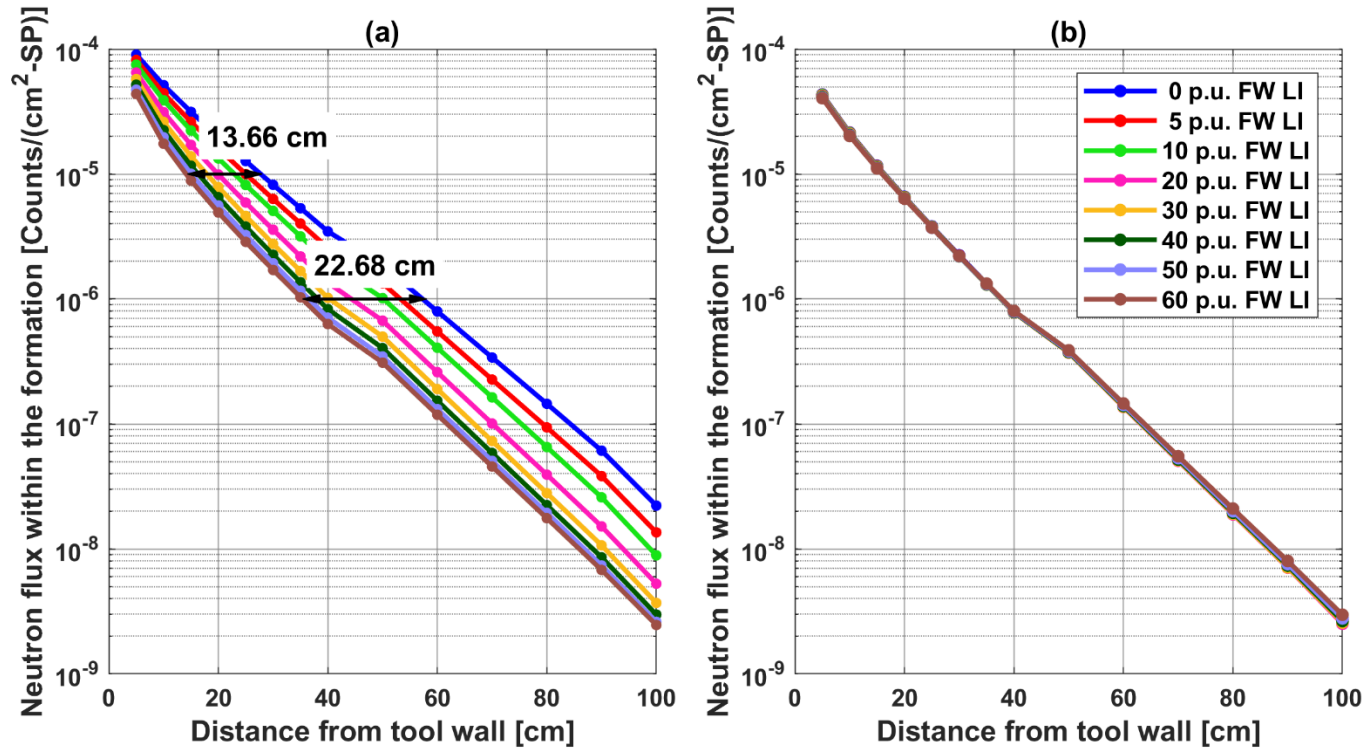


Figure 2.5. Cross-plot of neutron flux within the formation and radial distance from tool wall illustrating the spatial extent of the fast neutron cloud depending on hydrogen index (porosity) for neutrons with energies (a) between 1 and 4 MeV, and (b) between 4 and 14.1 MeV, in freshwater-filled limestone formations.

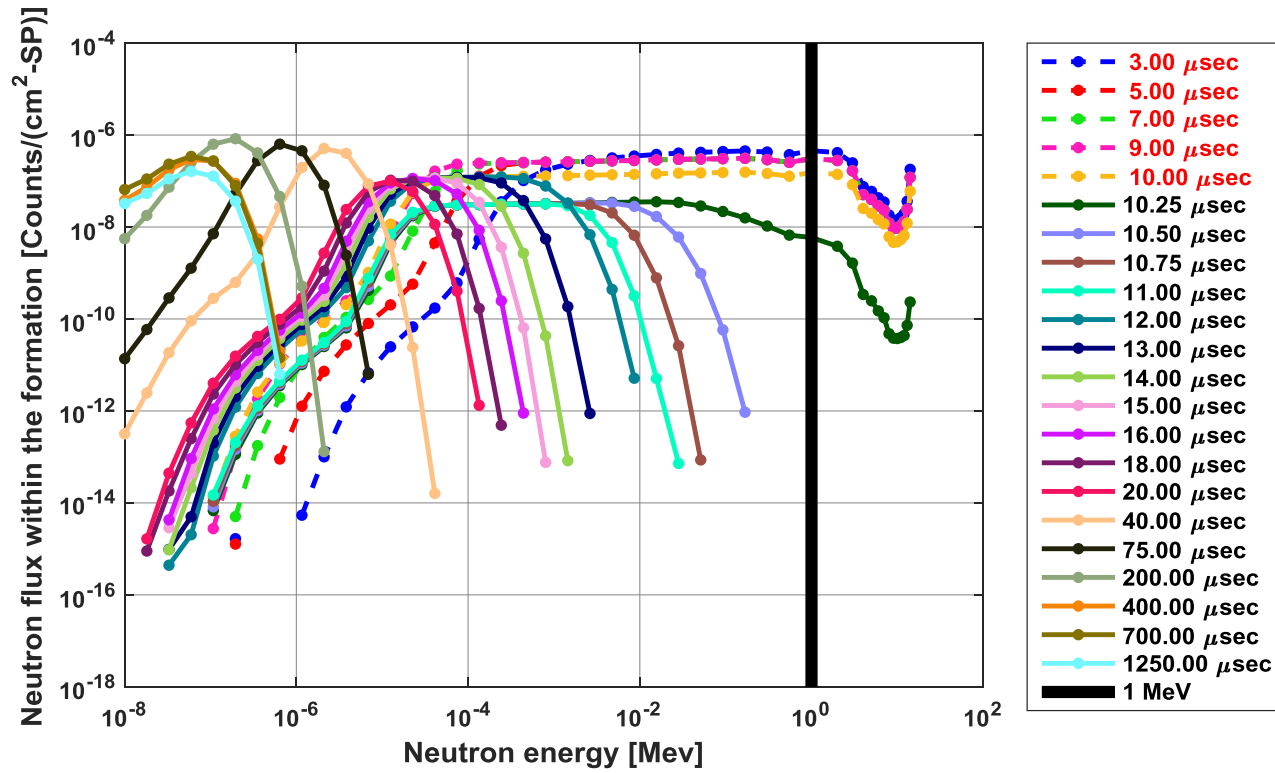


Figure 2.6. Neutron flux inside a 0 p.u. limestone block with respect to neutron energy at different time steps during (dashed lines) and after (solid lines) the burst. The black vertical line identifies a 1 MeV threshold below which inelastic scattering interactions are unlikely to occur.

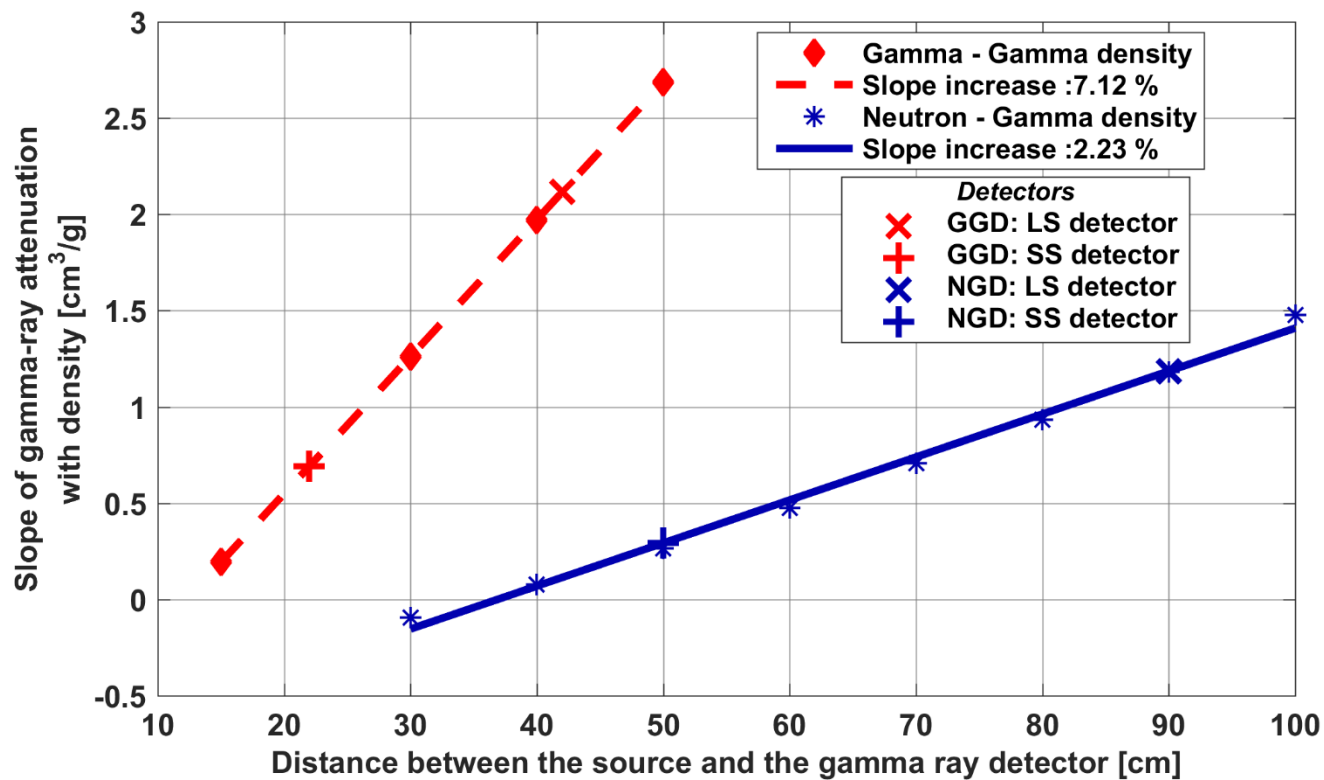


Figure 2.7. Slope of gamma-ray attenuation as a function of source-detector distance for Neutron-Gamma density and Gamma-Gamma density measurements. For reference, the positions of long- and short-spaced gamma-ray detectors in the Longhorn Gamma-Gamma density and Neutron-Gamma density tools are identified with cross and plus signs, respectively.

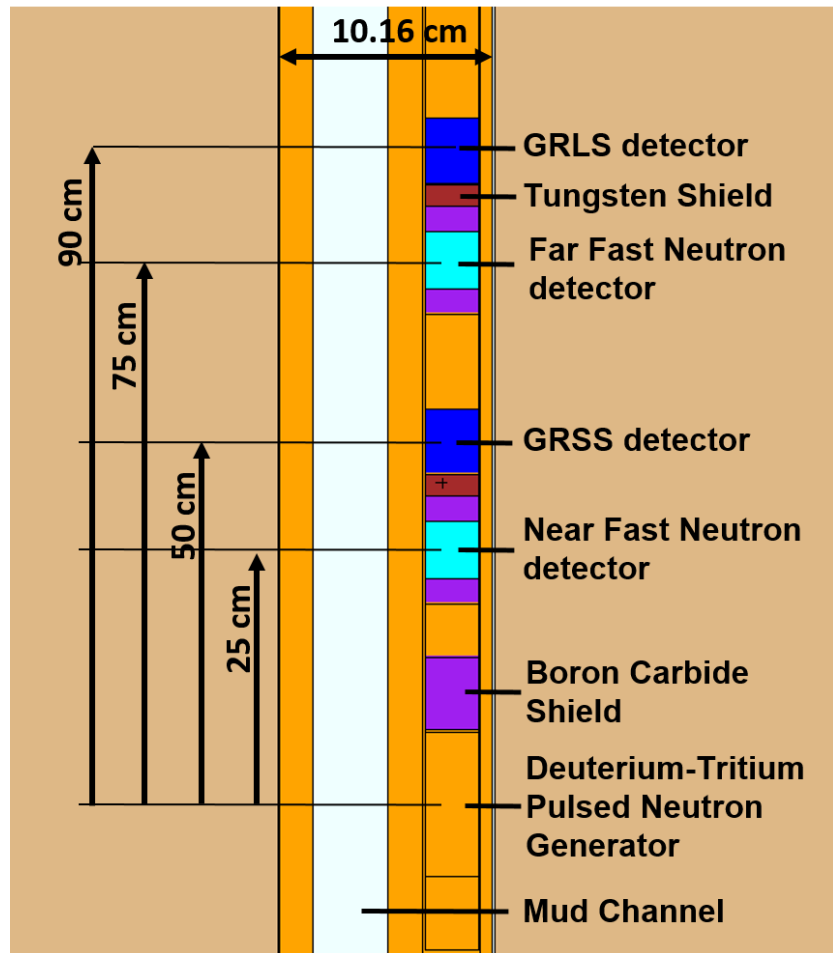


Figure 2.8. Schematic of the Longhorn logging-while-drilling (LWD) Neutron-Gamma density tool (Luycx and Torres-Verdín, 2017).

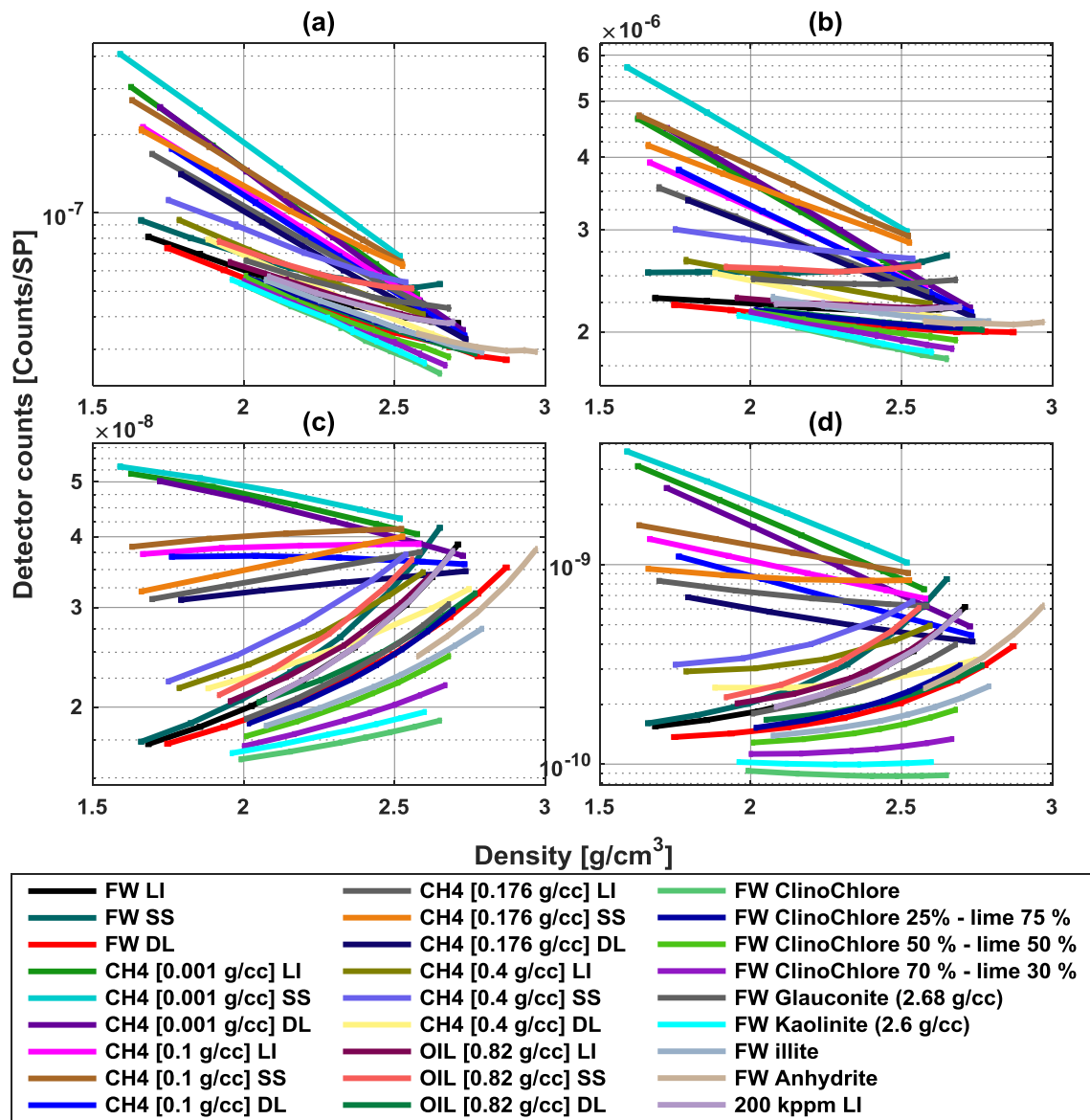


Figure 2.9. Detector counts of the Longhorn Neutron-Gamma density tool with respect to bulk density for common rock compositions at (a) long-spaced (GRLS) and (b) short-spaced (GRSS) gamma-ray detectors, and at (c) near (FastN) and (d) far (FastF) fast neutron detectors. MCNP modeling of fast neutron detectors includes a lower energy bin at 1 MeV.

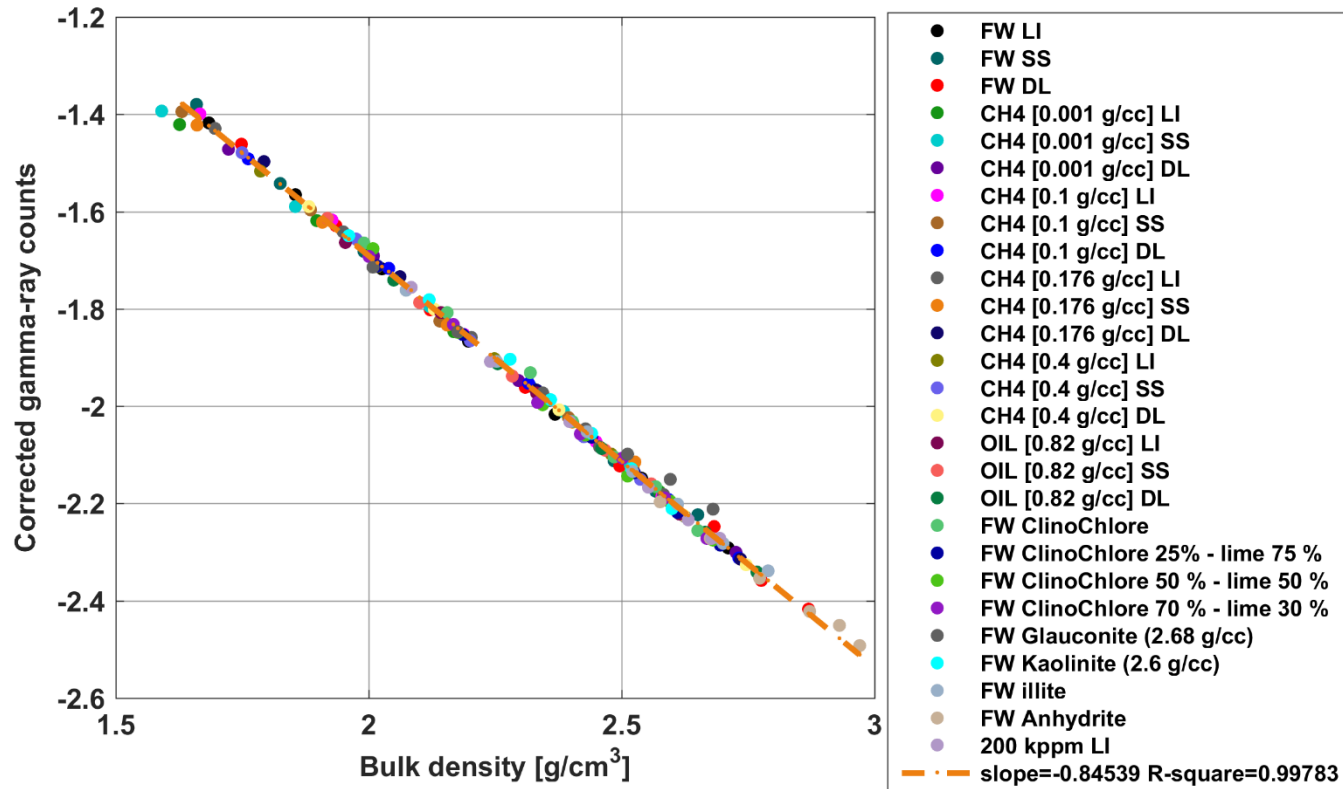


Figure 2.10. Cross-plot of corrected gamma-ray counts – calculated using the density estimation algorithm (equation 2.13) – and bulk density. Rock compositions listed in the legend are used as inputs for the inversion of unknown fitting coefficients a_i and m_1 in equation 2.13. FW stands for “freshwater-filled”, 200 kppm stands for “formation filled with 200 kppm NaCl water” (Luycx and Torres-Verdín, 2017).

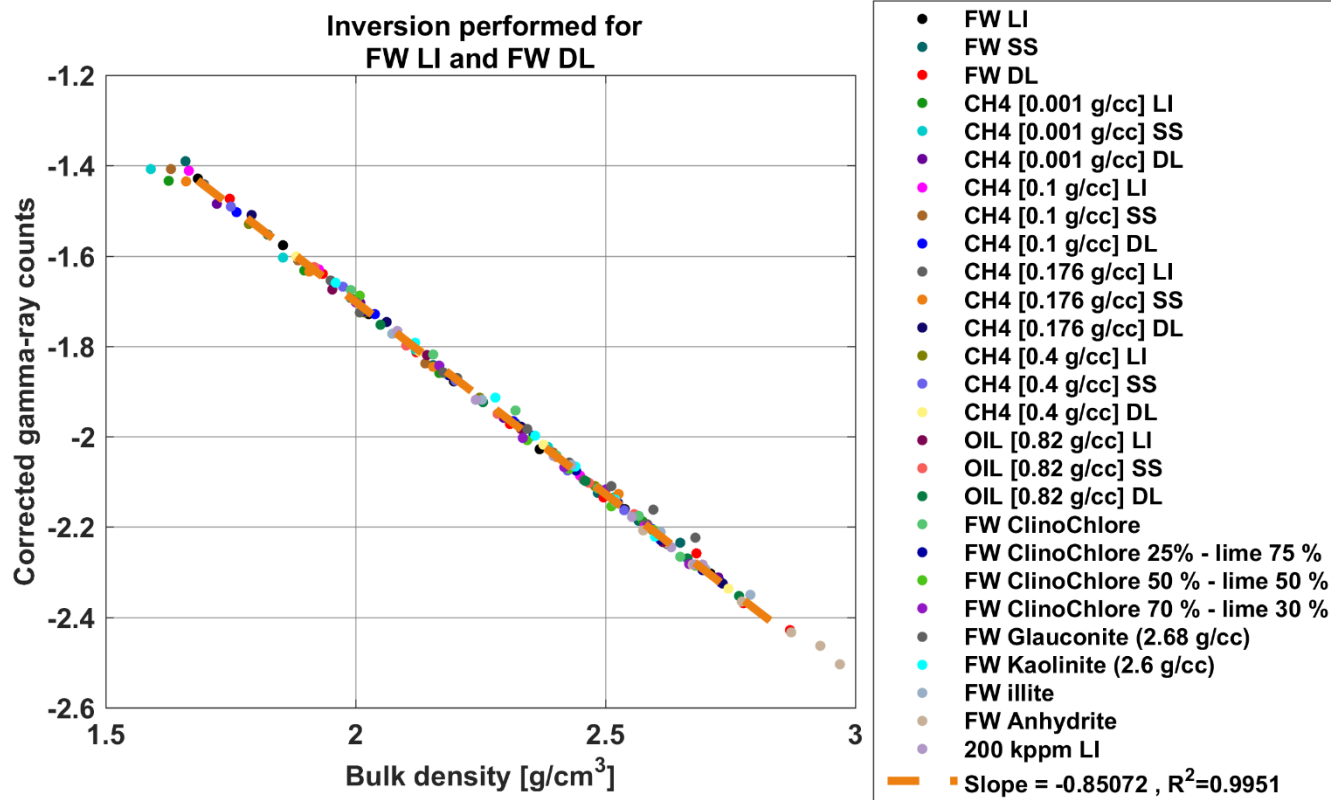


Figure 2.11. Cross-plot of corrected gamma-ray counts – calculated using the density estimation algorithm (equation 2.13) – and bulk density. Freshwater-filled limestone and dolomite formations are used as inputs for the inversion of unknown fitting coefficients a_i and m_1 in equation 2.13. FW stands for “freshwater-filled”, 200 kppm stands for “formation filled with 200 kppm NaCl water”.

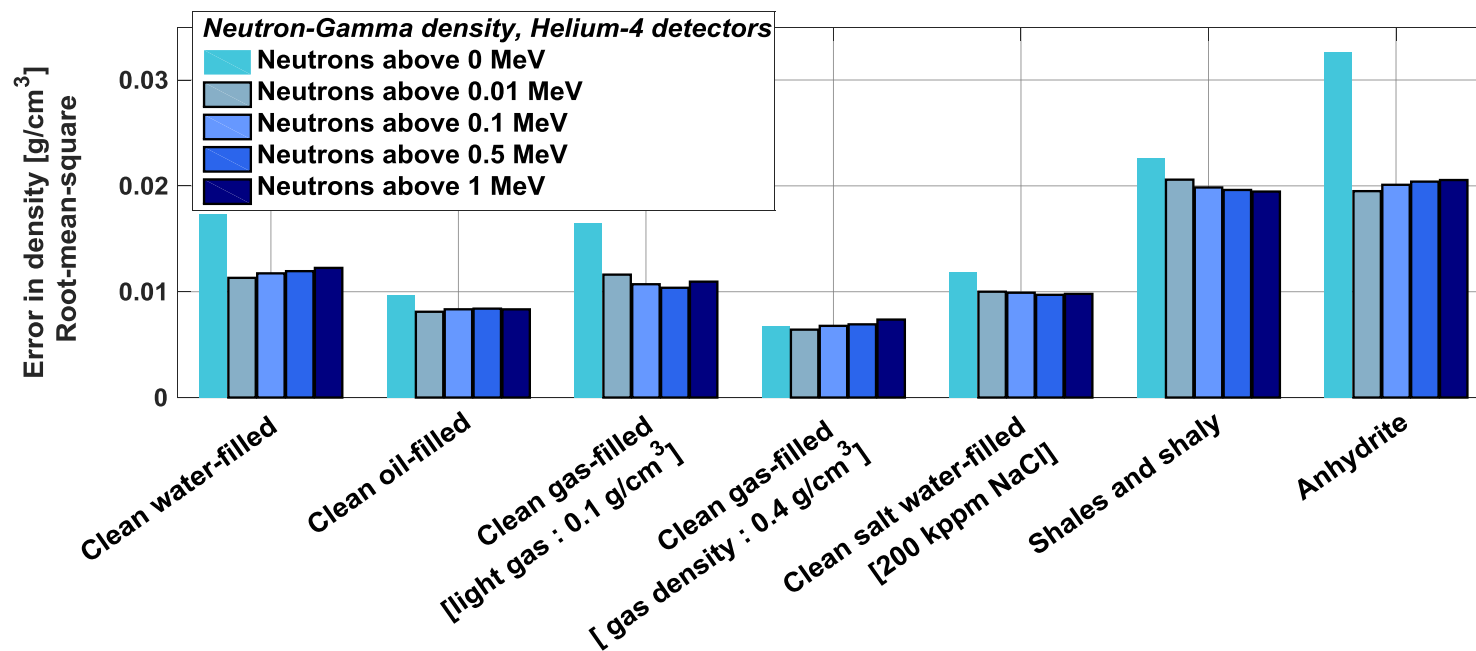


Figure 2.12. Comparison of root-mean-square density errors for the Longhorn Neutron-Gamma density tool across seven types of rock compositions, calculated using fast neutron counts from different energy ranges.

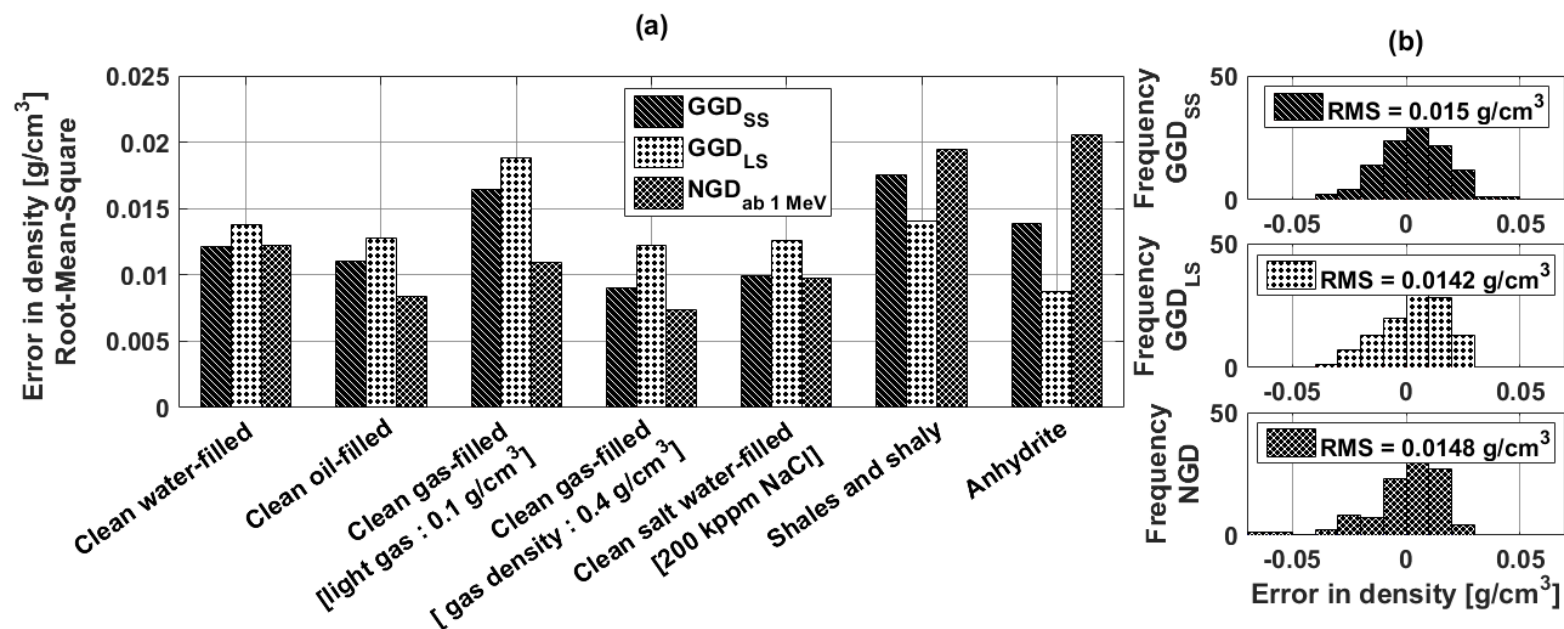


Figure 2.13. (a) Comparison of the density accuracy of the Longhorn Neutron-Gamma density and Gamma-Gamma density tools across seven types of rock compositions, and (b) overall density accuracy. RMS stands for root-mean-square.

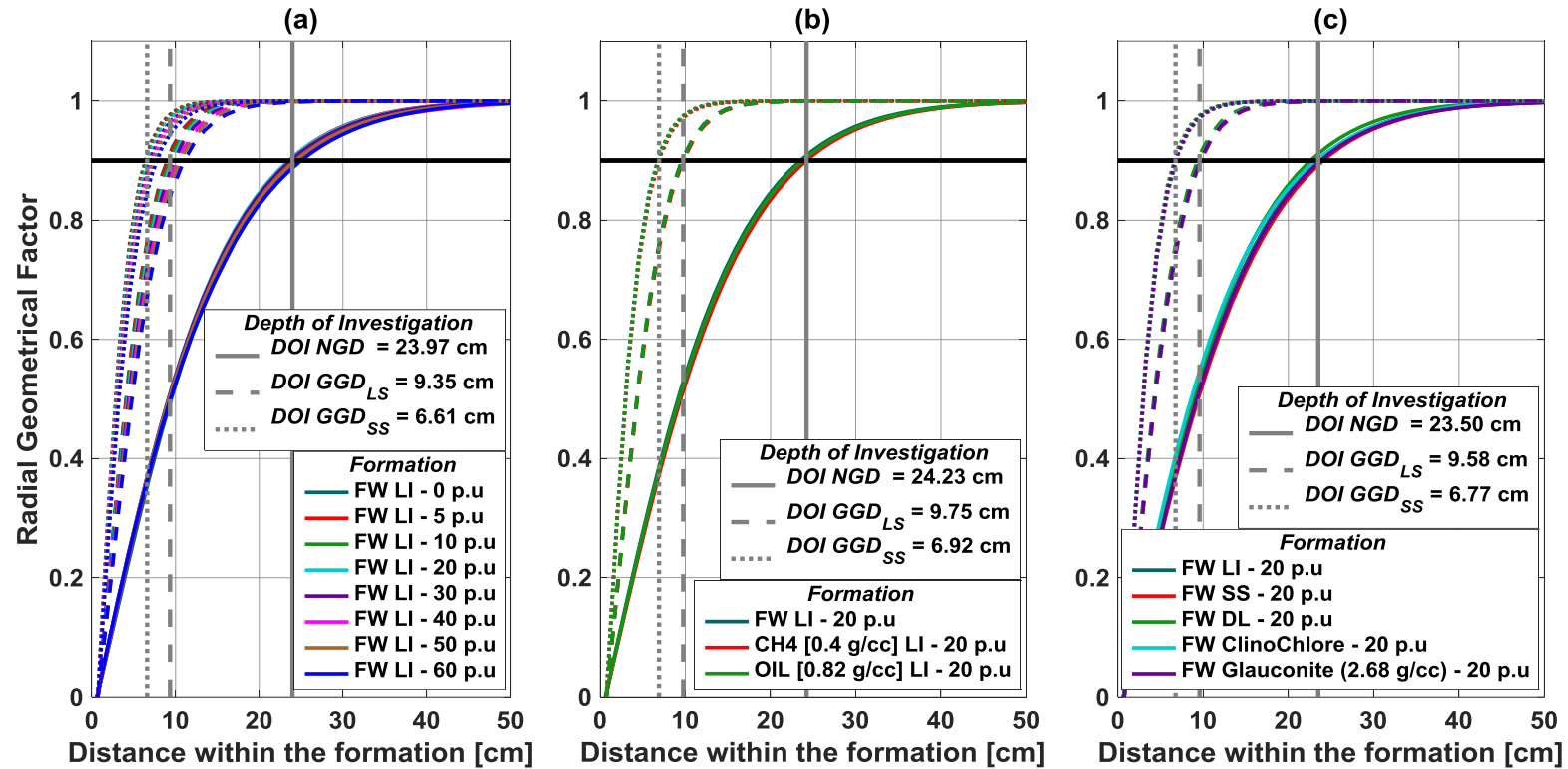


Figure 2.14. Depth of investigation (DOI) of Longhorn LWD Neutron-Gamma density and Gamma-Gamma density tools. Radial geometrical factor at the long-spaced gamma-ray detector for Neutron-Gamma density (solid lines), and at long- and short-spaced gamma-ray detectors for Gamma-Gamma density (dashed lines) for (a) different porosities, (b) different formation fluids, and (c) different lithologies.

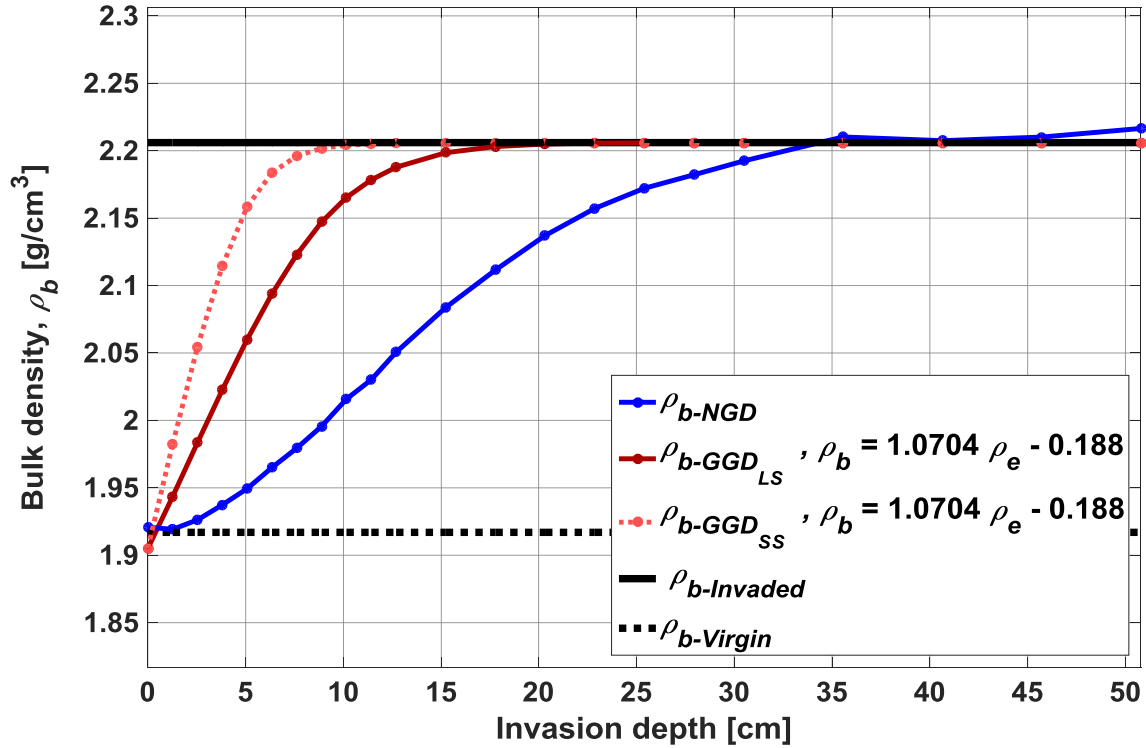


Figure 2.15. Comparison of simulated Neutron-Gamma density and Gamma-Gamma density measurements for a piston-like invasion of a 30 p.u. gas-filled ($\text{CH}_4 - 0.1 \text{ g/cm}^3$) limestone formation by 25 kppm NaCl water-base mud. Simulated density for the Longhorn LWD Neutron-Gamma density tool is identified with solid blue lines, simulated densities at long- and short-spaced detectors for the Longhorn LWD Gamma-Gamma density tool are identified with solid dark-red, and dashed light-red lines, respectively. Black dashed and solid lines identify bulk density of virgin and invaded zones, respectively.

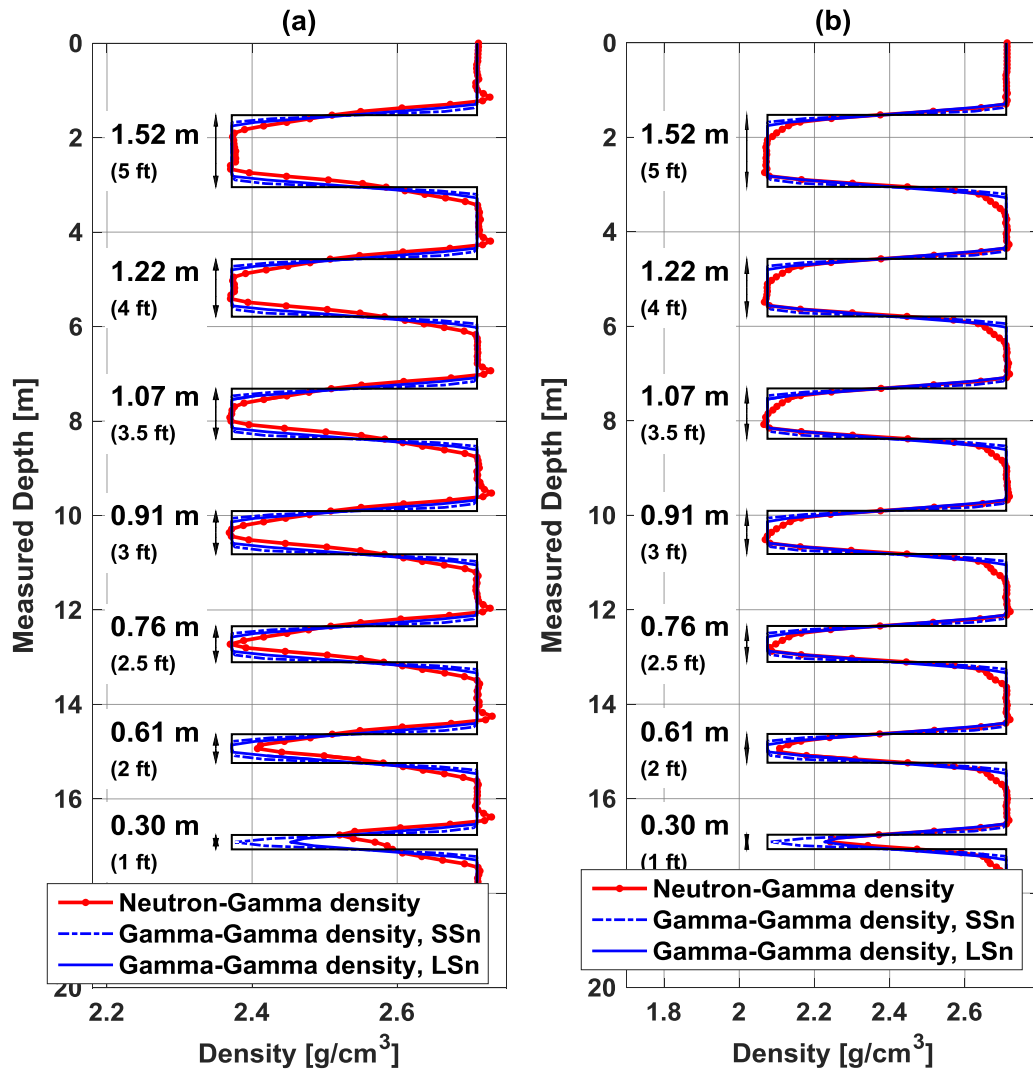


Figure 2.16. Comparison of the vertical resolution of Neutron-Gamma density and Gamma-Gamma density Longhorn tools in a vertical well. The background medium is a 0 p.u limestone block (2.71 g/cm³), while the layers are (a) fresh water-filled 20 p.u limestone (2.268 g/cm³), and (b) gas-filled (CH₄ - 0.2 g/cm³) 25 p.u limestone (2.0825 g/cm³).

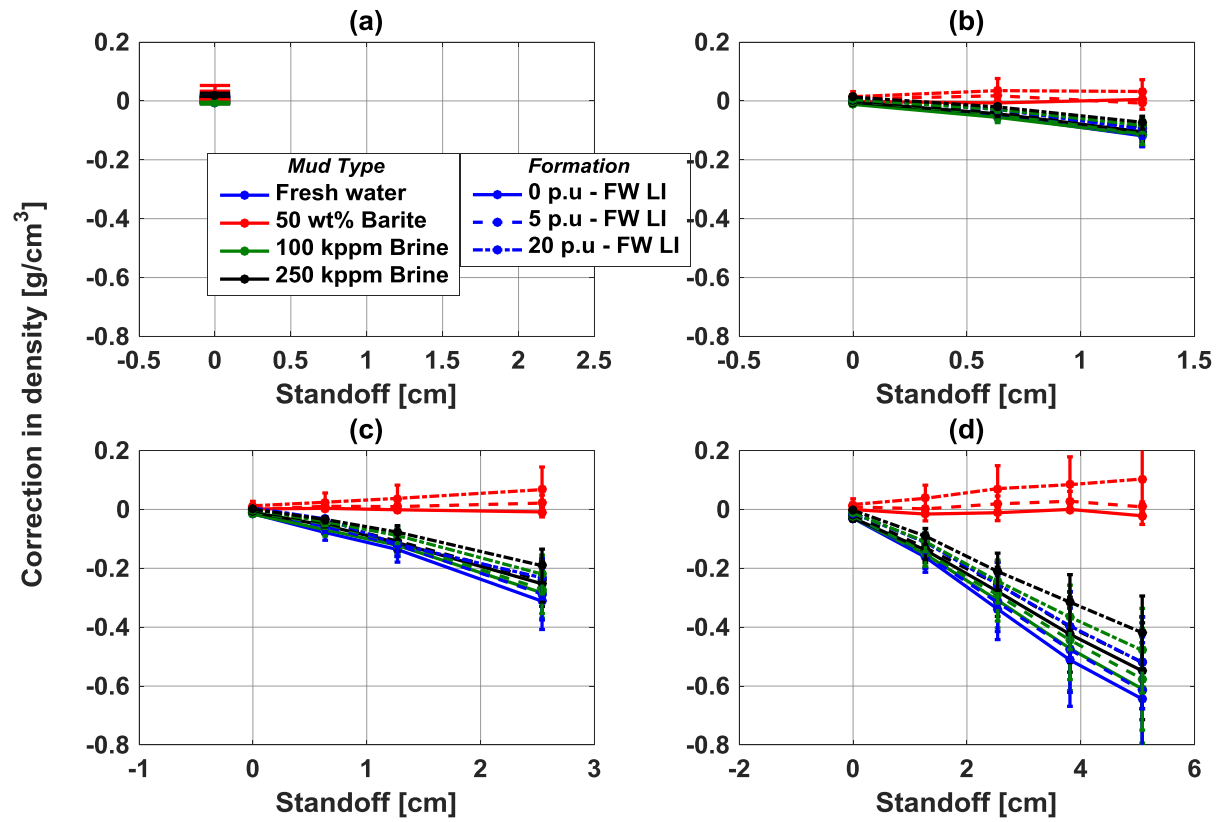


Figure 2.17. Effect of standoff on density correction for (a) 20-cm (8-in), (b) 22-cm (8.5-in), (c) 23-cm (9-in), and (d) 25-cm (10-in) boreholes (eccentered tool configuration) in fresh water-filled limestone formations, depending on mud type and formation porosity.

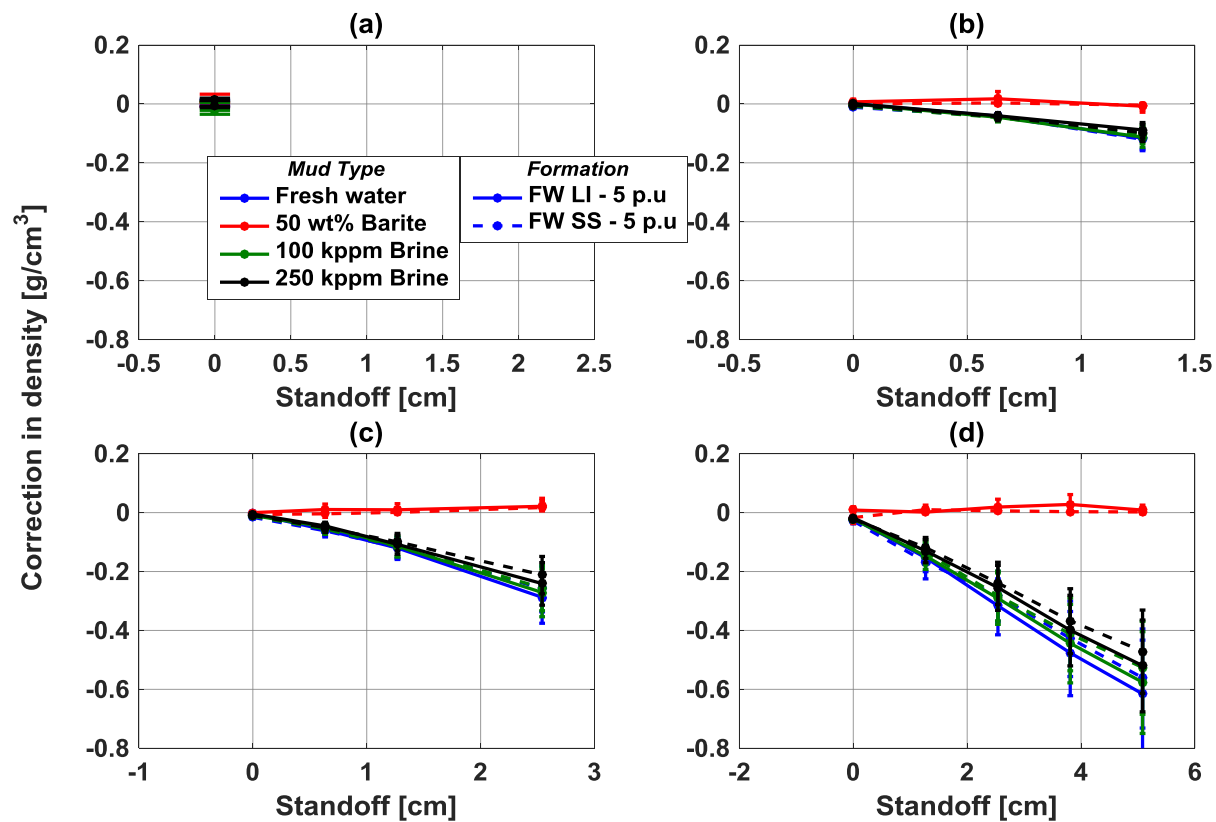


Figure 2.18. Effect of standoff on density correction for (a) 20-cm (8-in), (b) 22-cm (8.5-in), (c) 23-cm (9-in), and (d) 25-cm (10-in) boreholes (eccentered tool configuration) in 5 p.u. formations, depending on mud type and formation lithology.

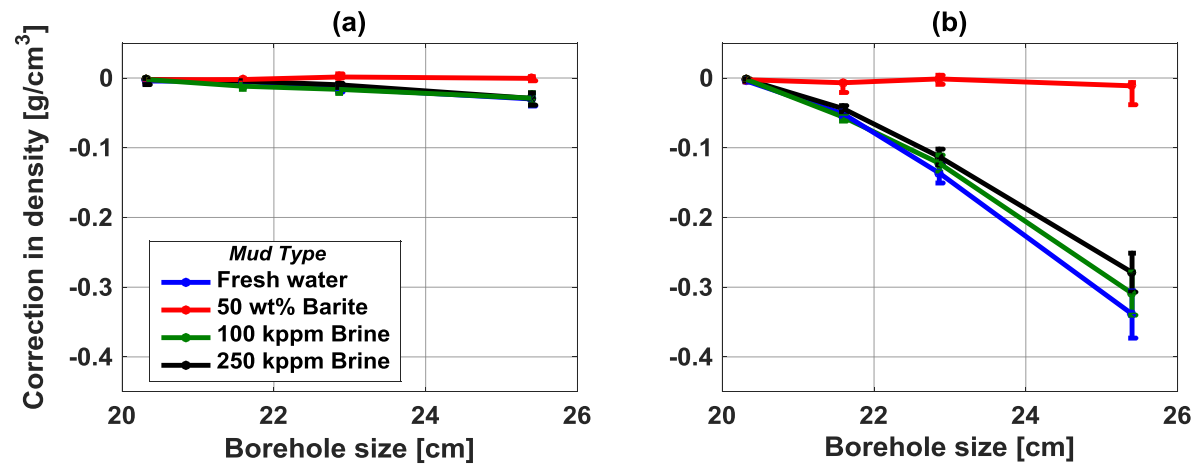


Figure 2.19. Effect of increasing borehole size on density correction with (a) eccentered, and (b) centered tool configurations in a 0 p.u. limestone formation, depending on mud type.

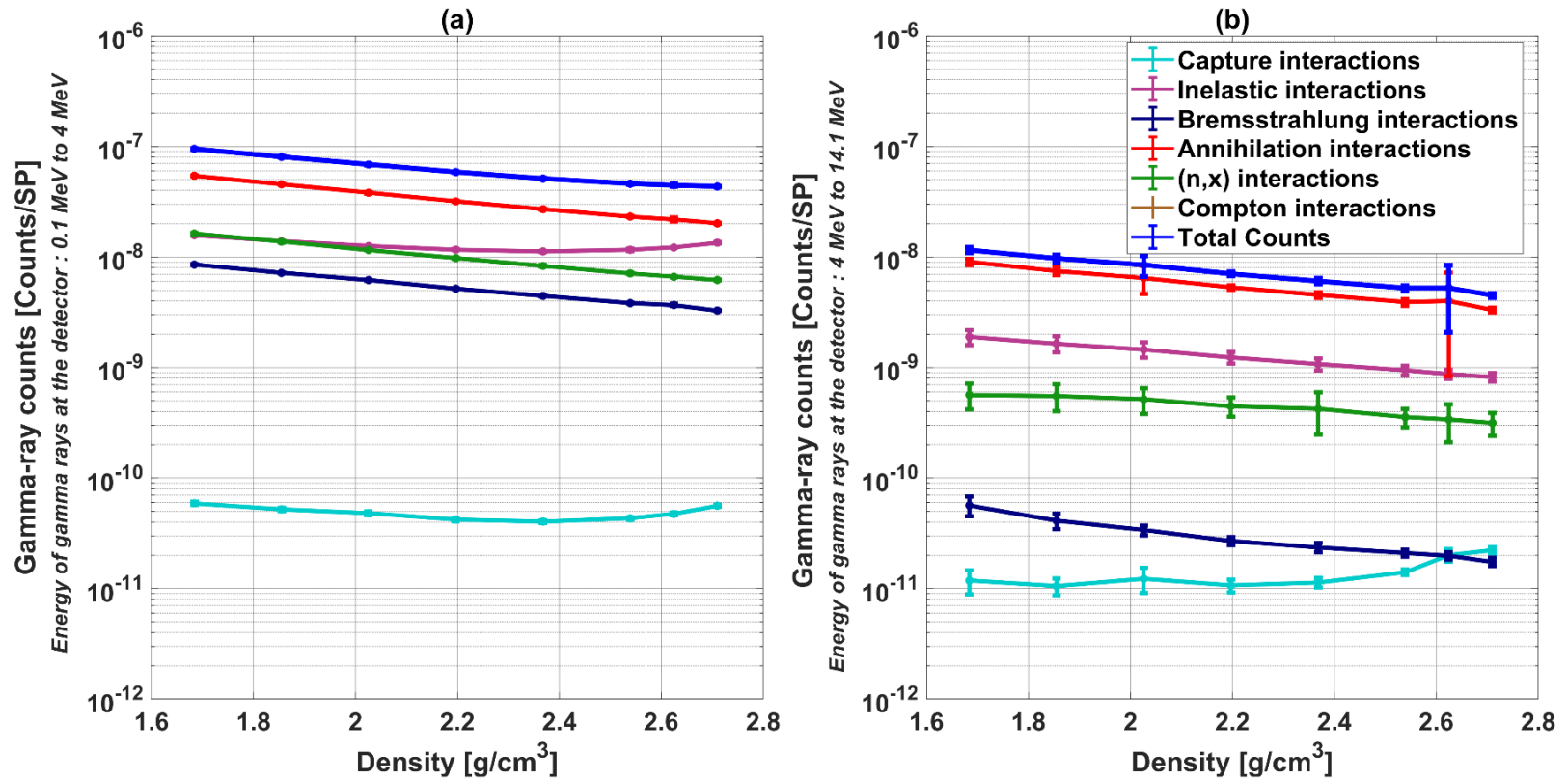


Figure 2.20. Analysis of nuclear interactions contributing to total Neutron-Gamma density gamma-ray counts considering the last production event (subsequent Compton scattering events are ignored) for gamma rays measured at the long-spaced detector (a) below 4 MeV and (b) above 4 MeV. (n,x) interactions include, for example, (n,2n), (n, α), (n,n' α), (n,p), (n,n'p) or (n,d) interactions.

Chapter 3: Rapid Forward Modeling of Logging-While-Drilling Neutron-Gamma Density Measurements

Neutron-activated gamma-ray (Neutron-Gamma) logging-while-drilling (LWD) measurements deliver bulk density estimates without using a chemical source. The assessment of bulk density is based on neutron-induced non-capture gamma rays, corrected for neutron transport by combining particle counts acquired at two gamma-ray detectors and two fast neutron detectors. Particle counts from all four detectors are necessary to deliver one density measurement whose accuracy compares well to that of Gamma-Gamma density instruments. Thereafter, borehole environmental effects are mitigated with empirical corrections based on Monte Carlo (MC) modeling. Such corrections should be avoided for standoff values greater than 0.63 cm (0.25 in) because they are no longer independent of formation properties. Neutron-Gamma density measurements are also influenced by bed-boundary and layer-thickness effects. Thinly-bedded formations, invasion, high-angle/horizontal (HA/HZ) wells, and enlarged boreholes can all mask true formation bulk density when implementing conventional petrophysical interpretation.

Although Monte Carlo methods accurately simulate three-dimensional (3D) environmental and geometrical effects, they are computationally expensive, and thus impractical for real-time interpretation. Layer-by-layer bulk density can, however, be estimated using rapid numerical simulations coupled with inversion procedures. I develop a rapid modeling algorithm to accurately simulate LWD

Neutron-Gamma density measurements. Simulations are based on a theoretical, albeit realistic LWD Neutron-Gamma density tool operating with a 14.1 MeV pulsed neutron source. The algorithm uses flux sensitivity functions and first-order Taylor series approximations to simulate particle counts at each detector before they are processed with a density estimation algorithm. Rigorous benchmarks against MCNP in vertical and HA/HZ wells, across diverse solid and fluid rock compositions, thin beds, and in the presence of invasion yield average density errors of less than 1% (0.023 g/cm^3) in approximately $5 \cdot 10^{-5}$ the time required with Monte Carlo modeling.

3.1 INTRODUCTION

Borehole Neutron-Gamma density measurements provide a non-radioactive alternative to borehole Gamma-Gamma density measurements. To accomplish that, the chemical gamma-ray source cesium-137 is replaced with a pulse neutron generator, and bulk density is estimated from neutron-activated, non-capture gamma-ray counts. Because non-capture gamma rays are generated when fast neutrons (with energy greater than 1 MeV) interact with formation nuclei, the secondary gamma-ray source is distributed within the formation in space, energy, and intensity (Inanc, 2014; Luycx and Torres-Verdín, 2018a). Most Neutron-Gamma density tools thus attempt to correct for the variability of the secondary gamma-ray source (in space, energy, and intensity) using fast, epithermal, or thermal neutron detectors.

The concept of measuring bulk density with neutron-activated gamma rays was first proposed by Wilson (1995). Odom et al. (2001) introduced a through-

casing Neutron-Gamma density tool where inelastic gamma-ray counts could be corrected for the variability of the secondary gamma-ray source (in space, energy, and intensity) using a single fast neutron detector. The first commercial Neutron-Gamma density tool was developed by Evans et al. (2012) and Reichel et al. (2012), making use of epithermal and thermal neutron detectors to compensate for neutron transport. In complex lithologies such as shales or anhydrite, Luycx and Torres-Verdín (2018a) showed that accuracies comparable to Gamma-Gamma density measurements could only be achieved with tool designs that included two fast neutron and two gamma-ray detectors.

Similar to other borehole nuclear measurements, conventional petrophysical interpretation of Neutron-Gamma density can deliver inaccurate results because of three-dimensional (3D) geometrical and borehole effects. Such effects can mask true formation properties across thinly-bedded formations, in high-angle/horizontal (HA/HZ) wells, in the presence of invaded beds, or in enlarged boreholes. Fast numerical simulations can be implemented with inversion-based interpretation algorithms to improve the petrophysical analysis of measurements acquired under such conditions (Sanchez-Ramirez et al., 2009; Heidari et al., 2012, 2013; Ajayi et al., 2015b; Ortega et al., 2017). For Neutron-Gamma density, these methods offer significant advantages because (1) shoulder-bed averaging effects are non-negligible due to the relatively low vertical resolution (76 cm or 2.5 ft) of the measurement, (2) the measurement delivers asymmetrical log responses at boundaries between beds exhibiting contrasting density and/or hydrogen index (HI), and (3) the measurement is very sensitive to borehole environmental effects because spine-and-rib compensation procedures are impractical (Luycx and Torres-Verdín, 2018a).

The concatenated physical processes of coupled neutron and gamma-ray transport are described by the Boltzmann equation (Lewis and Miller, 1984). In spatially complex environments, solutions to the transport equation can be best approximated using Monte Carlo (MC) methods, implemented with the Monte Carlo N-Particle code (MCNP, Goorley, 2014). The code offers sufficient flexibility and accuracy for investigating arbitrary logging environments, such as complex well trajectories and tool/borehole configurations. Monte Carlo methods are very effective during tool design and tool calibration phases (Evans et al., 2012; Reichel et al., 2012). They are, however, CPU-intensive and time-consuming, hence impractical for routine petrophysical analysis over long depth intervals.

Rapid numerical simulations of borehole nuclear measurements were originally based on diffusion approximations (Tittle, 1961; Tittman and Wahl, 1965), but lacked both accuracy and speed to simulate complex geological environments. Watson (1984) later introduced the concept of sensitivity functions whereby tool responses can be approximated with perturbation theory (Watson, 1984, 1992; Couët and Watson, 1993; Case et al., 1994). Mendoza et al. (2007) showed that first-order perturbation theory (Lewins, 1965; Greenspan, 1976) coupled with flux sensitivity functions (FSFs) is reliable, fast, and accurate when simulating nuclear measurements across diverse logging environments. Flux sensitivity functions quantify the relative change in detector counts resulting from a spatial perturbation in formation cross section within the volume of investigation of the tool. Assuming a background homogeneous medium of known characteristic cross section, the perturbed detector response is estimated with respect to the background tool response using pre-computed sensitivity functions. Fast-forward modeling algorithms based on FSFs and perturbation theory were developed for

Gamma-Gamma density (Zhou et al., 2009; Mendoza et al., 2010a; Luycx and Torres-Verdín, 2018b), neutron porosity (Mendoza et al., 2010a; Ijase et al., 2013a), Sigma (Ortega et al., 2014), and spectroscopy (Ajayi et al., 2015a) borehole nuclear measurements. They were successfully coupled with inversion procedures to improve petrophysical interpretation in spatially complex formations (Ijase et al., 2013b, 2014; Ortega et al., 2017).

Developing fast-forward modeling algorithms for Neutron-Gamma density measurements is key to improving petrophysical interpretation in enlarged boreholes; empirical corrections should be avoided for standoff greater than 0.64-cm (0.25-in) because they are no longer independent of formation properties. Fast-forward modeling can also mitigate interpretation errors caused by asymmetrical measurement responses at boundaries between layers with large density and/or HI contrast, or by layer-boundary and layer-thickness effects. Below, I introduce a new rapid forward numerical algorithm for Neutron-Gamma density measurements. It offers sufficient speed and accuracy to enable the development of inversion-based interpretation in complex 3D geometries and well trajectories.

3.2 METHODS

3.2.1 Neutron-Gamma Density Logging-While-Drilling (LWD) Measurements

The theoretical, albeit realistic Longhorn LWD Neutron-Gamma density tool considered in this chapter is 20.3 cm (8 in) in diameter and operates with a 14.1 MeV pulsed neutron source (Luycx and Torres-Verdín, 2018a). It includes two fast neutron detectors, at 35 and 75 cm (14 and 30 in) from the source (FastN and

FastF, respectively), and two lanthanum-bromide gamma-ray detectors, located 50 and 90 cm (20 and 35 in) from the source (GRSS and GRLS, respectively). At gamma-ray detectors, non-capture gamma-ray counts are modeled with MCNP using an energy cutoff for neutrons below 1 MeV, while fast neutron counts are measured at helium-4 detectors with a lower energy bin of 1 MeV, and no energy cutoff. Consequently, energy levels of interest to simulate Neutron-Gamma density measurements range from 1 to 14.1 MeV.

A density estimation algorithm calculates bulk density and provides density accuracies similar to those achieved by traditional Gamma-Gamma density measurements, i.e., 0.012 and 0.019 g/cm³ in shale-free, and in shale and shaly formations, respectively (Luycx and Torres-Verdín, 2018a). Compared to Gamma-Gamma density measurements, the Longhorn Neutron-Gamma density tool is more sensitive to borehole environmental effects, and delivers asymmetrical measurement responses at boundaries between beds exhibiting sharp contrasts in hydrogen index and/or density. The larger depth of investigation of Neutron-Gamma density measurements (associated with lower vertical resolution) also causes increased spatial averaging effects across thin beds.

3.2.2 Rapid Numerical Simulation

3.2.2.1 *Formulation of the Forward Approximation*

The Boltzmann equation, which describes neutron and gamma-ray transport, can be solved with Monte Carlo algorithms (Lewis and Miller, 1984). Such methods are flexible and accurate but computationally intensive. Consequently, they have limited practical applications because inversion-based interpretation of borehole nuclear measurements requires rapid forward modeling

algorithms. A solution to the Boltzmann transport equation can be approximated with a Taylor series expansion (Watson, 1984, 1992; Case et al., 1994). The perturbed detector response, N , at detector position $\mathbf{r}_R$ is expressed as a function of the nuclear interaction cross section, Σ , that controls a specific type of measurement, i.e.,

$$N(\mathbf{r}_R) = N_b(\mathbf{r}_R) + N_b(\mathbf{r}_R) \sum_{m=1}^{\infty} \int d\mathbf{r} \frac{1}{m!} \frac{d^m N}{d\Sigma^m}(\mathbf{r}_R, \mathbf{r}) \left(\frac{\Delta\Sigma(\mathbf{r})}{\Sigma_b} \right)^m, \quad (3.1)$$

where N_b is background (reference) detector response associated with a background homogeneous formation described with cross section Σ_b , and $\frac{1}{m!} \frac{d^m N}{d\Sigma^m}$

is the m -th order response sensitivity coefficient. The perturbation is defined by $\Delta\Sigma(\mathbf{r}) = \Sigma(\mathbf{r}) - \Sigma_b$, i.e., the difference between perturbed and background cross sections.

In equation 3.1, higher-order terms ($m > 1$) account for flux perturbation effects and can be neglected when the perturbation is small, i.e., $\Delta\Sigma \ll \Sigma_b$. Thereafter, detector response N is locally linearized by invoking the first term of the Taylor series expansion, such that,

$$N(\mathbf{r}_R) \approx N_b(\mathbf{r}_R) + N_b(\mathbf{r}_R) \int d\mathbf{r} FSF_b(\mathbf{r}_R, \mathbf{r}) \frac{\Delta\Sigma(\mathbf{r})}{\Sigma_b}, \quad (3.2)$$

where FSF_b is the first-order response sensitivity coefficient, also referred to as background flux sensitivity function, associated with the interaction cross section Σ_b and the detector response N_b .

3.2.2.2 *Perturbation Parameters*

In equation 3.2, the interaction cross section, Σ , also referred to as perturbation parameter, Fp , is defined by a unique predictive relationship with detector counts. Determining this parameter is straightforward for Gamma-Gamma density (bulk density, ρ_b), neutron porosity (migration length, L_m), Sigma (thermal-neutron absorption cross section, Σ_a), or spectroscopy (elemental absolute yields, y_{abst}) measurements. Conversely, for Neutron-Gamma density, I construct new parameters for each detector using average microscopic cross sections, $\bar{\sigma}$, defined by (Glasstone and Sesonske, 1994)

$$\bar{\sigma} = \frac{\int_{E_{lb}}^{E_{up}} dE \sigma(E) \psi(E)}{\int_{E_{lb}}^{E_{up}} dE \sigma(E)}, \quad (3.3)$$

where ψ is particle flux, σ is microscopic interaction cross section for particles of energy E , and E_{lb} and E_{ub} are lower and upper energy bounds, respectively. Particle flux, ψ , is calculated based on two different assumptions for neutron transport:

- [1] Neutron transport in a pure scatterer medium (medium 1), and
- [2] Neutron transport in a strong absorber medium (medium 2).

[1] In a nonabsorbing medium (medium 1), assuming a constant reaction rate within each energy bin, the neutron flux is given by (Glasstone and Sesonske, 1994)

$$\psi(E) = \frac{S}{E \xi \Sigma_T(E)}, \quad (3.4)$$

where S is source strength, Σ_T is total macroscopic cross section, and ξ is average logarithmic energy decrement. Upon substituting the expression for flux in equation 3.3, the average microscopic elastic cross section $\bar{\sigma}_{elastic1}^j$ between 1 and 14.1 MeV for mineral or fluid j , reduces to

$$\bar{\sigma}_{elastic1}^j = \frac{\int_1^{14.1} dE \sigma_{elastic}^j(E) \frac{1}{E \sigma_T^j(E)}}{\int_1^{14.1} dE \frac{1}{E \sigma_T^j(E)}}, \quad (3.5)$$

assuming neutron transport in medium 1 (pure scatterer), where σ_T^j is total microscopic cross section for mineral or fluid j .

[2] In a strong absorber medium (medium 2), the scattering cross section is zero, except for $E=E_s$, with $E_s=14.1$ MeV, the energy of the source. The absorption cross section is constant except at E_s , where it is zero. Neutron flux is then expressed as

$$\psi(E) = \frac{\psi(E_s) \Sigma_T(E_s) - S}{\Sigma_T(E)}. \quad (3.6)$$

By substituting neutron flux in equation 3.3 I obtain

$$\bar{\sigma}_{x2}^j = \frac{\int_1^{14.1} dE \sigma_x^j(E) \frac{1}{\sigma_T^j(E)}}{\int_1^{14.1} dE \frac{1}{\sigma_T^j(E)}}, \quad (3.7)$$

where $\bar{\sigma}_{x2}^j$, can be replaced with $\bar{\sigma}_{elastic2}^j$, the average microscopic elastic cross section, or by $\bar{\sigma}_{abs2}^j$, the average microscopic absorption cross section, assuming neutron transport in medium 2 (strong absorber).

Average macroscopic cross sections for mixtures of rocks and fluids, $\bar{\Sigma}$, are calculated with the mixing law

$$\bar{\Sigma} = \sum_j V^j \cdot N_d^j \cdot \bar{\sigma}_x^j, \quad (3.8)$$

where V^j is volumetric concentration of mineral or fluid j . Number density, N_d , is given by

$$N_d = \frac{\rho_b N_a}{M}, \quad (3.9)$$

where ρ_b is bulk density, N_a is Avogadro's number, and M is molecular mass. Neutron-Gamma density detector counts are also influenced by the hydrogen content index, Hc^j , of each mineral or fluid j , defined as,

$$Hc^j = \frac{\sum_{ielt \in j} \frac{v_{ielt}^j}{M_{ielt}}}{\sum_{ielt \in j} v_{ielt}^j}, \quad (3.10)$$

where v_{ielt}^j is number of atoms of the kind $ielt$ in mineral or fluid j , and M_{ielt} is atomic weight of element $ielt$. For common rock compositions, the hydrogen content index of the solid and fluid rock mixture is also calculated with equation 3.8 and is closely correlated with hydrogen index, HI , except when hydrogen index is zero (**Figure 3.1**). The impact of inelastic scattering interactions on the fast neutron population

is described by $N_d \cdot M = \frac{N_a \rho_b}{M} \cdot M$. This quantity is directly proportional to bulk density, ρ_b , and denotes that the probability of inelastic scattering increases in the presence of heavy nuclei.

To determine the relative contributions of average elastic and absorption macroscopic cross sections, hydrogen content index, and bulk density to perturbation parameters at fast neutron detectors, I consider the relationship

$$\begin{aligned} & \sum_{m=0}^2 k_m F p^m \\ &= \sum_{m=0}^2 k_m \left[(c_1 \cdot \bar{\Sigma}_{elastic1}^{c_2} + c_3 \cdot \bar{\Sigma}_{abs2}^{c_4} + c_5 \cdot \bar{\Sigma}_{elastic2}^{c_6} + c_7 \cdot Hc^{c_8}) \cdot \rho_b^{c_9} \right]^m, \quad (3.11) \\ &\approx \log_e(Fast) \end{aligned}$$

where Fp is perturbation parameter, and $Fast$ represents fast neutron counts. Fitting coefficients, c_i and k_m , are calculated by solving the nonlinear inverse problem

$$F \begin{bmatrix} c_1 \\ \vdots \\ c_i \\ \vdots \\ c_{itot} \\ k_0 \\ k_1 \\ k_2 \end{bmatrix} = \begin{bmatrix} \log_e(Fast_1) \\ \vdots \\ \log_e(Fast_k) \\ \vdots \\ \log_e(Fast_{ktot}) \end{bmatrix}, \quad (3.12)$$

where fast neutron counts are computed in $ktot$ commonly encountered rock compositions, and F represents the nonlinear forward operator (equation 3.11).

The number of fitting coefficients $itot$ is equal to 9 in equation 3.11. The inverse problem is solved using the Levenberg–Marquardt algorithm (Aster et al., 2005); coefficients c_i and k_m are listed in **Table 3.1** for each detector.

At gamma-ray detectors, inelastic gamma-ray counts, GR , are approximated with

$$\begin{aligned} & \sum_{m=0}^2 k_m Fp^m \\ &= \sum_{m=0}^2 k_m \left[(c_1 \cdot \bar{\Sigma}_{elastic1}^{c_2} + c_3 \cdot \bar{\Sigma}_{abs2}^{c_4} + c_5 \cdot \bar{\Sigma}_{elastic2}^{c_6} + c_7 \cdot Hc^{c_8}) \cdot \rho_b^{c_9} + c_{10} \cdot \rho_e \right]^m, \quad (3.13) \\ &\approx \log_e (GR) \end{aligned}$$

where $(c_1 \cdot \bar{\Sigma}_{elastic1}^{c_2} + c_3 \cdot \bar{\Sigma}_{abs2}^{c_4} + c_5 \cdot \bar{\Sigma}_{elastic2}^{c_6} + c_7 \cdot Hc^{c_8}) \cdot \rho_b^{c_9}$ is the secondary gamma-ray source term, and ρ_e is electron density, with $c_{10} \cdot \rho_e$ accounting for exponential gamma-ray attenuation. Fitting coefficients, c_1 to c_{10} and k_0 to k_2 , are calculated by solving the nonlinear inverse problem (equation 3.12), where the nonlinear forward operator, F , is given by equation 3.13 with $itot$ equal to 10. Values of fitting coefficients c_i and k_m are listed in **Table 3.1** for the Neutron-Gamma density Longhorn tool. **Figure 3.2** shows a cross-plot of MCNP detector counts and perturbation parameter, Fp , for each detector. The root-mean-square error (RMSE) is less than 2.3% across diverse solid and fluid rock compositions.

The simulated earth model is described by detector-specific perturbation parameters, Fp , calculated for fast neutron detectors with equation 3.11, and for gamma-ray detectors with equation 3.13. The impact of perturbations ΔFp on detector response N is derived from equation 3.2 and given by

$$N(\mathbf{r}_R) \approx N_b(\mathbf{r}_R) + N_b(\mathbf{r}_R) \int d\mathbf{r} F S F_b(\mathbf{r}_R, \mathbf{r}) \frac{\Delta F p(\mathbf{r})}{F p_b} . \quad (3.14)$$

3.2.2.3 *Flux Sensitivity Functions Library*

Flux sensitivity functions are calculated from 3D importance maps computed with a modified version of the MCNP forward-adjoint or weight-window generator (Booth and Hendricks, 1984). On one hand, importance maps at fast neutron detectors are based on neutrons with energy greater than 1 MeV, measured at helium-4 detectors in neutron transport mode. On the other hand, importance maps at gamma-ray detectors are constructed from fast neutrons, whose interactions with formation nuclei produce secondary gamma rays measured at lanthanum-bromide detectors in coupled neutron-photon transport mode. To differentiate between capture and non-capture gamma-rays, importance maps are also defined using an energy weight-window group corresponding to neutrons with energies greater than 1 MeV. Sensitivity functions are computed with 16 azimuthal sectors in the presence of the tool, formation, and borehole. Therefore, they account for borehole and geometrical effects caused by thin beds, dipping layers, and arbitrary well trajectories, across diverse solid and fluid rock compositions.

Because sensitivity functions at fast neutron and gamma-ray detectors are constructed based on fast neutron transport, the fast slowing-down length, L_{Fast} , is the best parameter to quantify sensitivity flux perturbations. The fast slowing-down length is calculated with UTNuPRO (University of Texas – Nuclear Properties), an algorithm that implements a revised Kreft's method (Kreft, 1974, Morstin and Kreft, 1983). Kreft's method is commonly employed to approximate neutron slowing-

down lengths to thermal energy levels, L_s , in homogeneous formations (McKeon and Scott, 1989). It was adapted to approximate neutron attenuation to fast energy levels (1 MeV), and compute neutron fast slowing-down lengths, L_{Fast} .

Homogeneous perturbations in sensitivity functions are governed by linear and uniform variations in neutron fast slowing-down length, as illustrated by **Figure 3.3**, where vertical sensitivity responses for diverse rock compositions are color-coded and organized with respect to L_{Fast} . **Figures 3.4 and 3.5** show sensitivity function libraries for each detector, integrated in the radial and azimuthal directions, and vertical and azimuthal directions, respectively. In environments with low fast slowing-down length, fast neutrons do not undergo inelastic scattering away from the source because they are likely to have lost energy rapidly and fallen below the inelastic scattering energy threshold. Such environments tend to generate more gamma rays away from the detector; therefore, sensitivity functions at gamma-ray detectors are asymmetrical and skewed toward the source (located at 45 cm or 18 in on the vertical axis in **Figure 3.4**). Sensitivity functions are selected at each depth with the linear iterative refinement (LIR) process developed by Mendoza et al. (2010a), also implemented for fast-forward modeling of borehole spectroscopy measurements (Ajayi et al., 2015a).

3.2.3 Density Estimation Algorithm

Detector counts simulated with MCNP and with the fast-forward algorithm are processed identically to compute bulk density, ρ_b . First, simulated detector counts are corrected for depth and resolution matching, where the vertical resolution of each detector is evaluated at 50% of their vertical geometrical factor, ZJ (Ijasan et al., 2011). Second, depth and resolution-matched detector counts are

processed using the density estimation algorithm of the Longhorn Neutron-Gamma density tool (Luycx and Torres-Verdín, 2017), given by

$$\rho_b = \frac{1}{m_1} \left[\log_e \left(\frac{GRLS}{GRSS} \right) - \sum_{i=0}^2 a_i \log_e \left(\frac{FastF}{FastN} \right)^i \right], \quad (3.15)$$

where *GRLS* and *GRSS* are gamma-ray counts at long- and short-spaced gamma detectors, respectively; *FastF* and *FastN* are fast neutron counts at far and near neutron detectors, respectively. Fitting coefficients m_1 and a_i are calculated by solving a linear inverse problem and are reported in Luycx and Torres-Verdín (2018a). It is also worth noting that rapid numerical simulations should yield density accuracies within the same order of magnitude than those of the density estimation algorithm (0.02 g/cm³ on average).

3.3 RESULTS

I benchmark the proposed fast-forward algorithm against Monte Carlo simulations using several challenging synthetic cases, including a vertical well with complex mineralogy, 45° and 85° deviated wells, thinly-bedded formations, and piston-like invasion. The misfit is estimated with respect to MC simulations using the root-mean-square error (RMSE). Maximum errors are also calculated at the 90-th percentile to disregard possible outliers resulting from MCNP simulation errors.

3.3.1 Vertical Well with Complex Mineralogy

Complex minerals are composed of certain elements such as aluminum (Al), chlorine (Cl), iron (Fe), and magnesium (Mg) whose elastic, absorption, and inelastic cross sections exhibit higher variability than oxygen (O), carbon (C), or calcium (Ca) between 1 and 14.1 MeV. Therefore, in formations with complex mineralogy, relationships between perturbation parameters and detector counts are challenged by the approximations applied when averaging cross sections over a large energy range (equation 3.3). Synthetic Case 1 examines the accuracy of the fast-forward algorithm along a vertical well in the presence of complex rock compositions, such as shale, shaly formations, and anhydrite. **Table 3.2** lists the layer properties assumed in this example, including true-stratigraphic-thickness (TST), rock composition, and bulk density. The fast-forward algorithm simulates detector counts (**Figure 3.6**) within 8.5% accuracy (error at the 90-th percentile) compared to MC methods. Panels (a) to (d) show FF (solid line) and MC counts (red circles) at long- and short-spaced gamma-ray detectors, and at near and far fast neutron detectors. Panel (e) describes the volumetric rock compositions listed in **Table 3.2**. Root-mean-square errors are 1.5, 1.0, 1.7, and 5% at the GRLS, GRSS, FastN, and FastF detectors, respectively. Simulated detector counts are processed using the density estimation algorithm to determine bulk density (**Figure 3.7a**). The difference between MC- and FF-derived bulk densities at the 90-th percentile is 0.035 g/cm^3 (1.44%), and the RMSE is 0.022 g/cm^3 (0.87%). I conclude that the fast-forward algorithm accurately simulates detector counts and bulk density in formations exhibiting complex mineralogy.

3.3.2 High-Angle Wells

In deviated wells, the effective volume of investigation for each detector is exposed to different sections of the layered formation as the LWD tool rotates azimuthally in the borehole. Hence, detectors with relatively longer depth of investigation tend to sense bed boundaries earlier than those with relatively shorter depth of investigation. Such effects are non-negligible for Neutron-Gamma density measurements because detector counts acquired at four detectors, with depth of investigations ranging from 13 cm (5.1 in) to 24 cm (9.4 in), deliver one density measurement.

Synthetic Cases 2 and 3 study the measurement response for 45° and 85° deviated wells, respectively. Layer properties for Synthetic Case 2 are listed in **Table 3.3**. **Figure 3.8** shows resolution-matched, FF simulated, detector counts at the bottom (180°), left (90°), and top (0°) sectors. Fast-forward counts at the bottom sector are compared to Monte Carlo simulations and yield accuracies (90-th percentile) within 2.8, 0.8, 1.2, and 4.3% at the GRLS, GRSS, FastN, and FastF detectors, respectively. Root-mean-square errors are 2.2, 0.5, 0.9, and 3%, respectively. After processing, the FF-simulated density log compares well to Monte Carlo calculations within 0.030 g/cm³ (1.17%) at the 90-th percentile, and RMSE is 0.023 g/cm³ or 0.95% (**Figure 3.9**). Coupled neutron and gamma-ray transport can cause higher-order effects across regions of significant contrasting properties. For example, gamma-ray long-spaced detector counts exhibit a nonlinear response with respect to formation bulk density at 6.7 m (22 ft) in measured depth (**Figure 3.8a**). The fast neutron source is located in a high-porosity formation (30 p.u. freshwater-filled dolomite), whereas the gamma-ray detector operates in a low-porosity, high-density medium. Fast neutron counts are

thus negatively impacted by the presence of hydrogen, while gamma rays undergo strong attenuation within the high-density bottom layer. This combined effect causes a decrease in gamma-ray counts at the bed boundary. Because this fast-forward algorithm is based on first-order approximations, such behavior, which is caused by higher-order effects (in the form of sensitivity flux perturbations), cannot be accurately simulated. Consequently, the FF-simulated density log (**Figure 3.9**) at the bed boundary located at 6.5 m (21.2 ft) does not match the MC-simulated measurement response. At this depth, fast modeling errors are as high as 0.07 g/cm³. However, it is worth noting that such measurement responses only occur at boundaries between layers exhibiting large contrasts in formation properties (in this case, porosity decreased sharply by 30%). Nonlinear measurement responses (with respect to formation bulk density) are also observed at 2.4 m (8 ft), and 4.7 m (15.5 ft) in **Figure 3.9**. Rather than being caused by flux perturbations, they originate from each detector having different vertical resolutions and depth of investigations, as shown in **Figure 3.8**. In this case, the fast-forward algorithm accurately simulates the asymmetrical tool response and helps to mitigate interpretation errors.

Synthetic Case 3, described in **Table 3.4**, examines an 85° well penetrating a typical siliciclastic reservoir with transitions from water, to oil, and to gas-filled formations. **Figure 3.10** compares MC and FF density logs simulated at the bottom sector. The fast-forward algorithm yields density accuracy within 0.032 g/cm³ (1.21%) at the 90-th percentile, and RMSE is 0.022 g/cm³ or 0.86%. Because hydrogen-index and density contrasts between layers are less significant here than in Synthetic Case 2, measurement responses are linear (with respect to formation bulk density) across bed boundaries. The fast-forward algorithm accurately

simulates the 3D geometrical effects caused by the relative angle between well axis and formation dip plane.

3.3.3 Thinly-Bedded Formations

In thinly-bedded formations, inversion-based interpretation algorithms can be implemented to subtract spatial averaging effects and infer true layer-by-layer bulk densities. The vertical resolution of Neutron-Gamma density was estimated to be 76 cm (30 in) (Luycx and Torres-Verdín, 2017). Synthetic Cases 4A, 4B, and 4C study Neutron-Gamma density measurements across 61-cm (24-in), 30.5-cm (12-in), and 15-cm (6-in) laminated beds, respectively. **Table 3.5** describes the layered siliciclastic formation composed of 5 p.u. shale (80% clinochlore and 20% illite) interbedded with 20 p.u. freshwater-filled sandstone (SS). The fast-forward algorithm simulates the impact of shoulder-bed effects for each detector according to their vertical resolution. Detector counts are then processed with the density estimation algorithm to compute bulk density logs (**Figures 3.11 to 3.13**). In each case, density logs are smoothed over the sequence, increasingly so as layer thickness decreases. Rapid numerical simulations yield density accuracy of 0.024 g/cm³ (0.98%) at the 90-th percentile, and root-mean-square error of 0.014 g/cm³, or 0.55% for 61-cm (24-in) laminations (**Figure 3.11**). With 30.5-cm (12-in) laminations, the difference between MC- and FF-derived densities is 0.025 g/cm³ (0.98%) at the 90-th percentile, and RMSE is 0.016 g/cm³ or 0.65% (**Figure 3.12**). Finally, when the measurement is acquired across 15-cm (6-in) layers, the fast numerical simulation yields 0.031 g/cm³ (or 1.17%) accuracy at the 90-th percentile, and a root-mean-square error of 0.017 g/cm³ or 0.65% (**Figure 3.13**). Rapid numerical simulations based on flux sensitivity functions accurately simulate

geometrical effects across layers with thicknesses below the vertical resolution of the tool. The fast-forward algorithm can be efficiently combined with inversion-based interpretation across thin beds because its accuracy compares well to that achieved by the density estimation algorithm.

3.3.4 Presence of Invasion

Invasion by mud filtrate produces flux perturbations in the radial direction. Nonetheless, the fast-forward algorithm accurately quantifies the impact of invasion on Neutron-Gamma density measurements because spatial sensitivity flux perturbations are sufficiently small to have negligible impact. **Figure 3.14** compares MC and FF densities for an axis-symmetrical piston-like radial invasion profile, where 100 kppm NaCl brine invades a 30-p.u. gas-bearing ($0.1 \text{ g/cm}^3 \text{ CH}_4$) limestone formation. The difference between FF and MC simulated densities is 0.021 g/cm^3 (1.09%) at the 90-th percentile, and RMSE is 0.015 g/cm^3 or 0.62%. Maximum misfit occurs for an invasion radius of 5 to 15 cm (2 and 6 in), where sensitivity to radial flux perturbations is maximal.

3.4 DISCUSSION

3.4.1 Higher-Order Effects

Across bed boundaries exhibiting large contrasts in hydrogen index and/or density, Neutron-Gamma density measurements can be affected by higher-order effects (with respect to the perturbation parameter, Fp). Such behavior cannot be accurately reproduced by the fast-forward algorithm, which is based on first-order approximations. In this section, I study the limitations of the fast-forward algorithm at bed boundaries (vertical perturbations), and at the borehole wall (radial

perturbations), two conditions that give rise to significant sensitivity flux perturbations.

3.4.1.1 *Vertical Flux Perturbations at Bed Boundaries*

In the presence of coupled neutron, and gamma-ray transport, **Figures 3.8 and 3.9** show the impact of flux perturbations at boundaries between beds with contrasting properties. These flux perturbations cannot be reproduced with first-order approximations, leading to maximum misfits of 0.07 g/cm^3 at 6.7 m (22 ft) in **Figure 3.9**. **Figure 3.15** replicates the conditions of the same bed boundary and compares fast neutron sensitivity functions at the long-spaced gamma-ray detector in homogeneous (dashed black line) and heterogeneous (solid blue line) formations. The top layer, where the source is located, is 30 p.u. freshwater-filled dolomite, while the bottom layer, which holds the GRLS detector, is a 0 p.u. limestone block. Elastic scattering with hydrogen usually causes sufficient energy loss for fast neutrons to fall below the energy levels required for inelastic scattering interactions. Consequently, the heterogeneous sensitivity function is skewed toward the source because the measured gamma-rays originate from fast neutrons emitted in high-HI environments that promptly undergo inelastic scattering, before losing energy through elastic scattering with hydrogen. Such flux perturbations can be predicted qualitatively but cannot be estimated quantitatively using first-order perturbations with respect to background homogeneous sensitivity functions. Methods were developed to quantify flux perturbations at bed boundaries for Sigma (Mimoun et al., 2011), and neutron porosity (Ijase et al., 2013a) measurements. However, the latter approaches were focused on quantifying

thermal-neutron flux perturbations with one-group diffusion approximations, and they would have to be modified for two-particle transport.

3.4.1.2 *Radial Flux Perturbations at the Borehole Wall*

Flux perturbations also occur in the radial direction, at the borehole wall when borehole mud and formation exhibit contrasting properties. Gamma rays are more likely to undergo photoelectric absorption in high-density (high-Z) materials, prompting a relative increase in gamma-ray sensitivity flux upon entering low-density (low-Z) media, such as enlarged freshwater-filled boreholes (**Figure 3.16**). The fast-forward algorithm implements first-order linear perturbation theory and does not have sufficient accuracy to quantify flux perturbations at the borehole wall. Because flux perturbations are limited when standoff is small, the FF algorithm yields errors lower than 0.015 g/cm^3 in the presence of 1.27-cm (0.5-in) standoff (22.9-cm borehole, centered tool configuration, **Figure 3.17a**). However, as borehole size increases, flux perturbations can no longer be approximated using linear interpolations of homogeneous FSFs, and the misfit at the 90-th percentile increases to 0.037 g/cm^3 for a 2.54-cm (1-in) standoff, and 0.084 g/cm^3 for a 5.08-cm (2-in) standoff (**Figure 3.17b, and 17c**). Diffusion (Ijasan et al., 2013a) and point-kernel (Luycx and Torres-Verdín, 2018b) approximations were introduced to simulate neutron, and Gamma-Gamma density measurements, respectively, to quantify radial and vertical flux perturbations caused by higher-order effects. To improve modeling accuracy at bed boundaries and at the borehole wall, similar techniques could be implemented for fast modelling of measurements based on coupled neutron and gamma-ray transport, such as Neutron-Gamma density.

3.4.2 Computational speed

The fast-forward simulations were executed on a Windows® PC, with an Intel® Core™ i7-7700HQ (2.80-GHz) processor, and Monte Carlo simulations were completed with a parallelized version of MCNP611 (Goorley, 2014) on Lonestar5, a Linux® cluster in the Texas Advanced Computing Center operating with 1252 Cray XC40 computer nodes, each with two 12-core Intel® Xeon® processing cores. **Table 3.6** summarizes CPU times required for each synthetic case, with root-mean-square and 90-th percentile errors calculated in percent, and in density. On average (RMSE), the fast-forward modeling algorithm simulates Neutron-Gamma density measurements within 0.023 g/cm³ or 1% error compared to MCNP calculations, while being approximately 500,000 times faster.

3.5 CONCLUSIONS

I developed a fast-forward modeling algorithm for LWD Neutron-Gamma density measurements. The algorithm is based on libraries of detector-specific spatial sensitivity functions, pre-calculated using MCNP. Particle counts are simulated independently for each detector and processed with a density estimation algorithm to compute bulk density.

Cross section parameters such as migration length or electron density do not exhibit bijective correlations (i.e., one-to-one correspondence) to fast neutron and non-capture gamma-ray detector counts across diverse rock compositions because nuclear interactions contributing to Neutron-Gamma density are complex and occur at energy levels above 1 MeV. New perturbation parameters are constructed using cross section averaging methods between 1 and 14.1 MeV such

that they exhibit a bijective correlation to detector counts independently of rock composition.

The linear perturbation theory used in the algorithm struggles to account for sensitivity flux perturbations arising across bed boundaries with large contrasts in hydrogen-index and/or density. Such flux perturbations are non-negligible in enlarged boreholes: although the fast-forward modeling algorithm achieves 0.015 g/cm³ accuracy up to 1.27-cm (0.5-in) standoff with freshwater mud, errors are greater than 0.02 g/cm³ for larger values of standoff.

Nonetheless, extensive benchmarks showed that the fast-forward algorithm yields average density accuracy below 0.023 g/cm³ compared to Monte Carlo simulations, in $5 \cdot 10^{-5}$ the CPU time required by MCNP. In challenging cases involving complex mineralogy and high-angle/horizontal wells, the algorithm delivers average density accuracies below 0.023 g/cm³ and maximum density errors of 0.035 g/cm³ at the 90-th percentile. In formations with 30.5-cm (1-ft) laminations, spatial averaging effects cause well logs to misrepresent density estimates by 0.1 g/cm³ in sand layers. Conversely, fast-forward and Monte Carlo simulated Neutron-Gamma density measurements agree within 0.016 g/cm³ on average.

The fast-forward algorithm possesses sufficient speed and accuracy to be combined with inversion-based interpretation workflows. Along arbitrary well trajectories and across complex mineralogy, thin beds, and standoff below 1.27 cm (0.5 in), 3D geometrical and borehole effects can be numerically simulated, and mitigated with inversion procedures to determine true layer-by-layer formation bulk density.

	GRLS	GRSS	FastF	FastN
<i>Fp</i>	$Fp = (c_1 \cdot \bar{\Sigma}_{elastic1}^{c_2} + c_3 \cdot \bar{\Sigma}_{abs2}^{c_4} + c_5 \cdot \bar{\Sigma}_{elastic2}^{c_6} + c_7 \cdot Hc^{c_8}) \cdot \rho_b^{c_9} + c_{10} \cdot \rho_e$		$Fp = (c_1 \cdot \bar{\Sigma}_{elastic1}^{c_2} + c_3 \cdot \bar{\Sigma}_{abs2}^{c_4} + c_5 \cdot \bar{\Sigma}_{elastic2}^{c_6} + c_7 \cdot Hc^{c_8}) \cdot \rho_b^{c_9}$	
<i>c</i>₁	-7.783	-0.016	343.901	29.884
<i>c</i>₂	0.007	0.973	4.099	0.021
<i>c</i>₃	0.305	0.976	8.274	3.974
<i>c</i>₄	0.048	0.696	1.494	2.191
<i>c</i>₅	5.306	1.213	-958.327	-29.433
<i>c</i>₆	0.046	0.772	4.219	0.011
<i>c</i>₇	4.380	3.454	0.805	0.626
<i>c</i>₈	0.005	0.003	0.484	0.383
<i>c</i>₉	0.034	-0.006	-0.140	0.841
<i>c</i>₁₀	0.130	0.037		
<i>k</i>₀	-1.97	-0.87	20.72	0.60
<i>k</i>₁	-0.51	-0.31	-12.57	-6.00
<i>k</i>₂	-7.96	0.33	-16.14	-21.11

Table 3.1. Fitting coefficients of the Longhorn Neutron-Gamma density tool for computing the perturbation parameter *Fp* at each detector.

Layer	TST [m]	Layer composition [v/v]		Bulk density, ρ_b [g/cm ³]
I	1.52	1	LI	2.7100
II	1.52	0.95 0.05	DL H2O	2.7765
III	1.52	0.5 0.4 0.1	SS Illite H2O	2.5410
IV	1.52	1	Anhydrite	2.9700
V	1.52	0.5 0.3 0.1 0.1	SS Kaolinite Clinochlore Oil (CH1.7805, 0.82 g/cm ³)	2.4520
VI	1.52	0.55 0.4 0.05	Illite Kaolinite H2O	2.6245
VII	1.52	0.65 0.2 0.15	LI Kaolinite CH4 (0.1 g/cm ³)	2.2965
VIII	1.52	1	LI	2.7100

Table 3.2. Layer properties of the earth model corresponding to Synthetic Case 1, shown in **Figures 3.6 and 3.7**. TST stands for true-stratigraphic-thickness, LI for limestone, SS for sandstone, and DL for dolomite.

Layer	TST [m]	Layer composition [v/v]		Bulk density, ρ_b [g/cm ³]
I	1.52	1	LI	2.7100
II	1.52	0.9 0.1	LI H2O	2.5390
III	1.52	0.9 0.1	LI CH4 (0.1 g/cm ³)	2.4490
IV	1.52	0.7 0.3	DL H2O	2.3090
V	1.52	1	LI	2.7100

Table 3.3. Layer properties of the earth model corresponding to Synthetic Case 2, featuring a 45° deviated well, and shown in **Figures 3.8 and 3.9**. TST stands for true-stratigraphic-thickness, LI for limestone, and DL for dolomite.

Layer	TST [m]	Layer composition [v/v]		Bulk density, ρ_b [g/cm ³]
I	1.22	1	LI	2.7100
II	1.22	0.72	Illite	2.5858
		0.18	Clinochlore	
		0.1	H2O	
III	1.22	0.9	SS	2.3950
		0.1	CH4 (0.1 g/cm ³)	
IV	1.22	0.72	Illite	2.5858
		0.18	Clinochlore	
		0.1	H2O	
V	1.22	0.9	SS	2.4670
		0.1	Oil (CH1.7805, 0.82 g/cm ³)	
VI	1.22	0.72	Illite	2.5858
		0.18	Clinochlore	
		0.1	H2O	
VII	1.22	0.8	SS	2.3200
		0.2	H2O	
VIII	1.22	0.72	Illite	2.5858
		0.18	Clinochlore	
		0.1	H2O	
IX	1.22	1	LI	2.7100

Table 3.4. Layer properties of the earth model corresponding to Synthetic Case 3, featuring an 85° deviated well, and shown in **Figure 3.10**. Shale matrix composition is 80% illite and 20% clinochlore. TST stands for true-stratigraphic-thickness, LI for limestone, and SS for sandstone.

Layer	Layer composition [v/v]		Bulk density, ρ_b [g/cm ³]
I	0.76	Illite	2.6739
	0.19	Clinochlore	
	0.05	H2O	
II	0.8	SS	2.3200
	0.2	H2O	

Table 3.5. Layer properties of the earth model corresponding to Synthetic Cases 4A, 4B, and 4C, featuring thinly-bedded formations, and shown in **Figures 3.11 to 3.13**. LI stands for limestone.

Case	Measurement points	CPU time		Root-mean-square error (RMSE)		Error at the 90 th percentile	
		MCNP (bottom sector) [days]	FFM [s]	[g/cm ³]	%	[g/cm ³]	%
1	81 x 16 sectors	1226	138	0.022	0.87	0.035	1.44
2	71 x 16 sectors	1072	108	0.023	0.95	0.030	1.17
3	69 x 16 sectors	1042	139	0.022	0.86	0.032	1.21
4A	73 x 16 sectors	1102	341	0.014	0.55	0.024	0.98
4B	77 x 16 sectors	1163	362	0.016	0.65	0.025	0.98
4C	55 x 16 sectors	830	227	0.017	0.65	0.031	1.17
5	22	21	8.75	0.015	0.62	0.021	1.09

Table 3.6. Comparison of CPU times, root-mean-square errors (RMSE), and 90th percentile errors achieved with MC and FF models for each synthetic case.

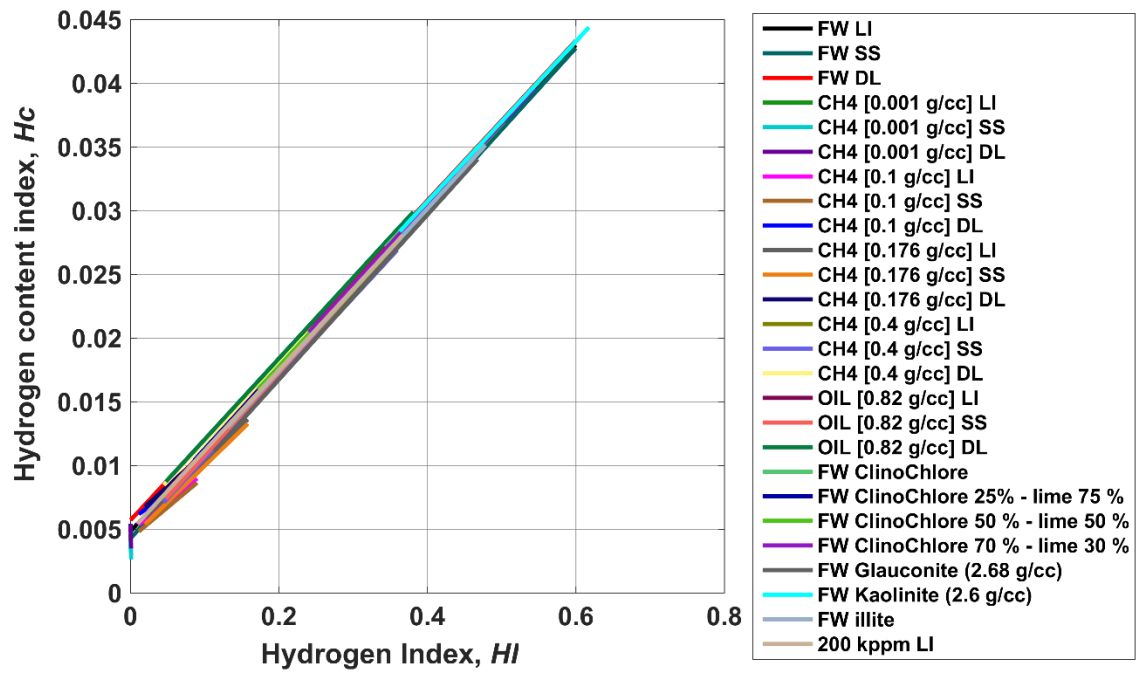


Figure 3.1. Cross-plot of hydrogen content index, H_c , and hydrogen index, HI , for common rock compositions. LI stands for limestone, SS, for sandstone, DL, for dolomite, FW, for freshwater, and 200 kppm, for “formation filled with 200 kppm NaCl brine”.

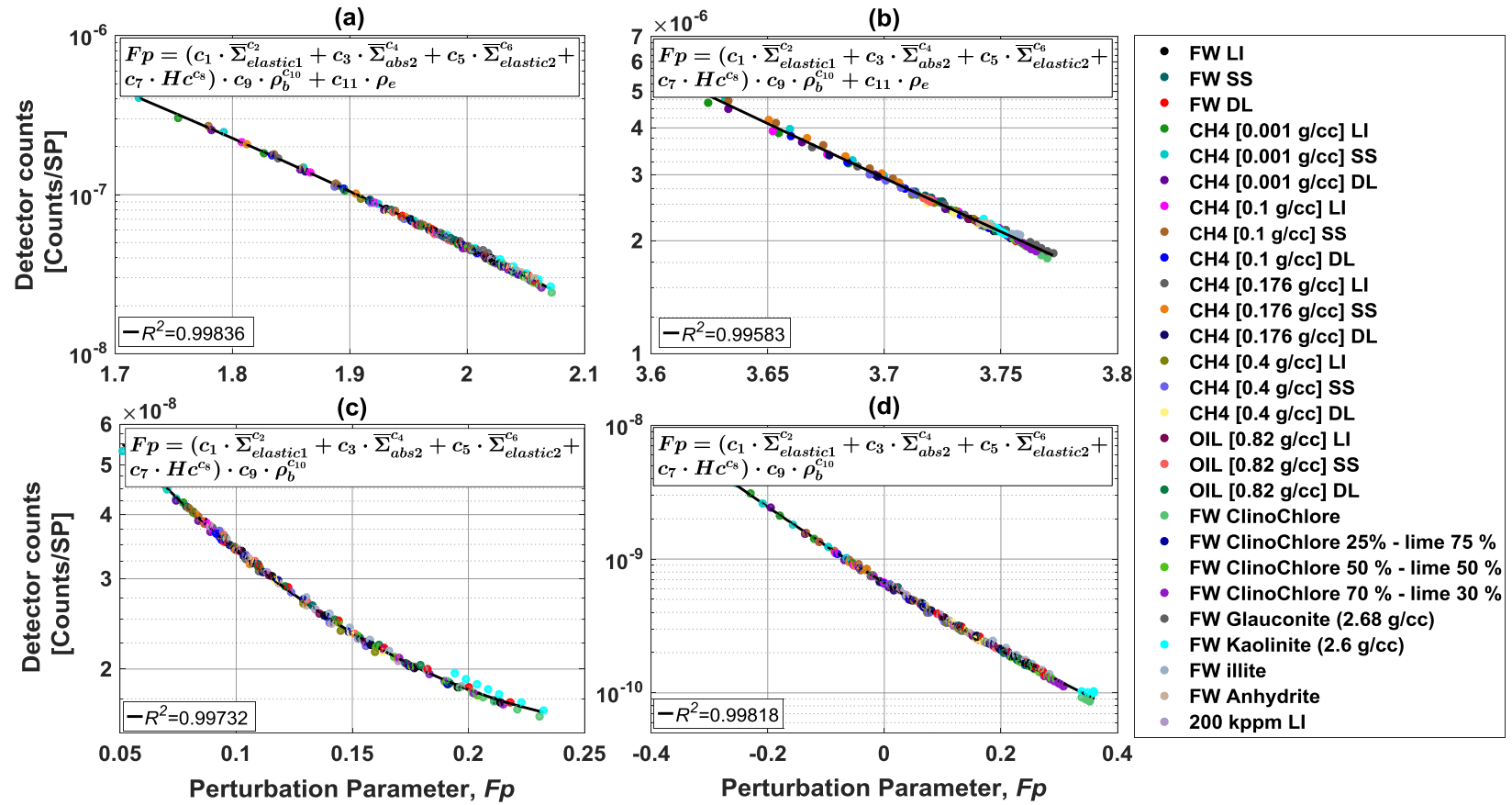


Figure 3.2. Cross-plot of MCNP detector counts and perturbation parameter, Fp , at (a) long- and (b) short-spaced gamma-ray detectors, and at (c) near and (d) far fast neutron detectors. The equations for Fp and the corresponding indicators of the goodness of fit, R^2 , are identified in each panel. Fitting coefficients, c_i and k_m , are listed in **Table 3.1**. LI stands for limestone, SS, for sandstone, DL, for dolomite, FW, for freshwater, and 200 kppm, for “formation filled with 200 kppm NaCl brine”.

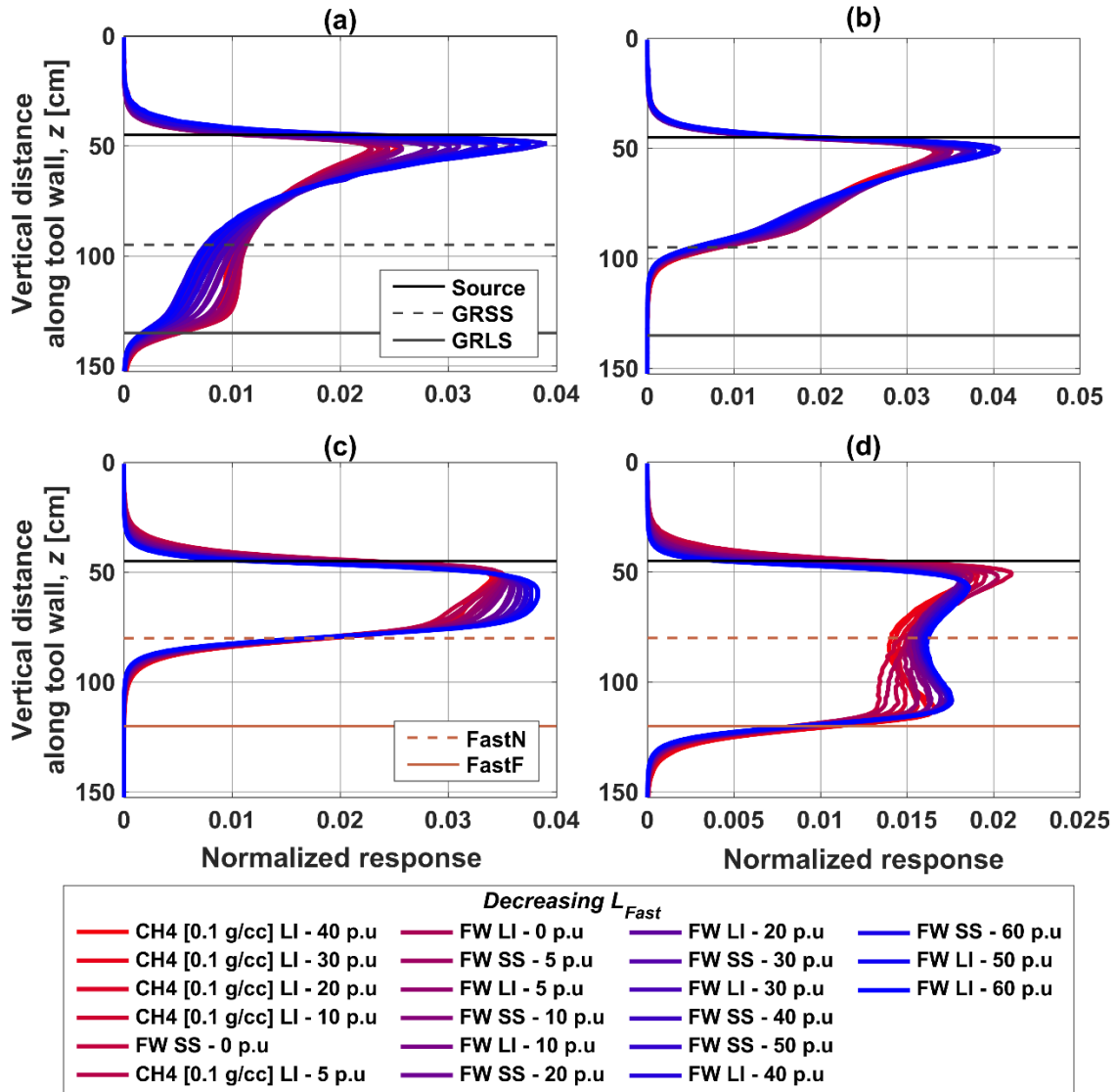


Figure 3.3. Impact of decreasing fast slowing-down length on neutron sensitivity functions integrated in the radial and azimuthal directions at (a) long- and (b) short-spaced gamma-ray detectors, (c) near and (d) far fast neutron detectors. The transition from red to blue denotes a decrease in fast slowing-down length, L_{Fast} , across diverse solid and fluid rock compositions. Solid black line at 45 cm (18 in) indicates the position of the pulsed neutron source, and the grey lines at 95 cm (37 in, solid line) and 135 cm (53 in, dashed line) indicate the location of short-, and long-spaced gamma-ray detectors, respectively. The locations of the near and far fast neutron detectors at 80 and 120 cm (31 and 47 in) are identified by dashed and solid brown lines, respectively.

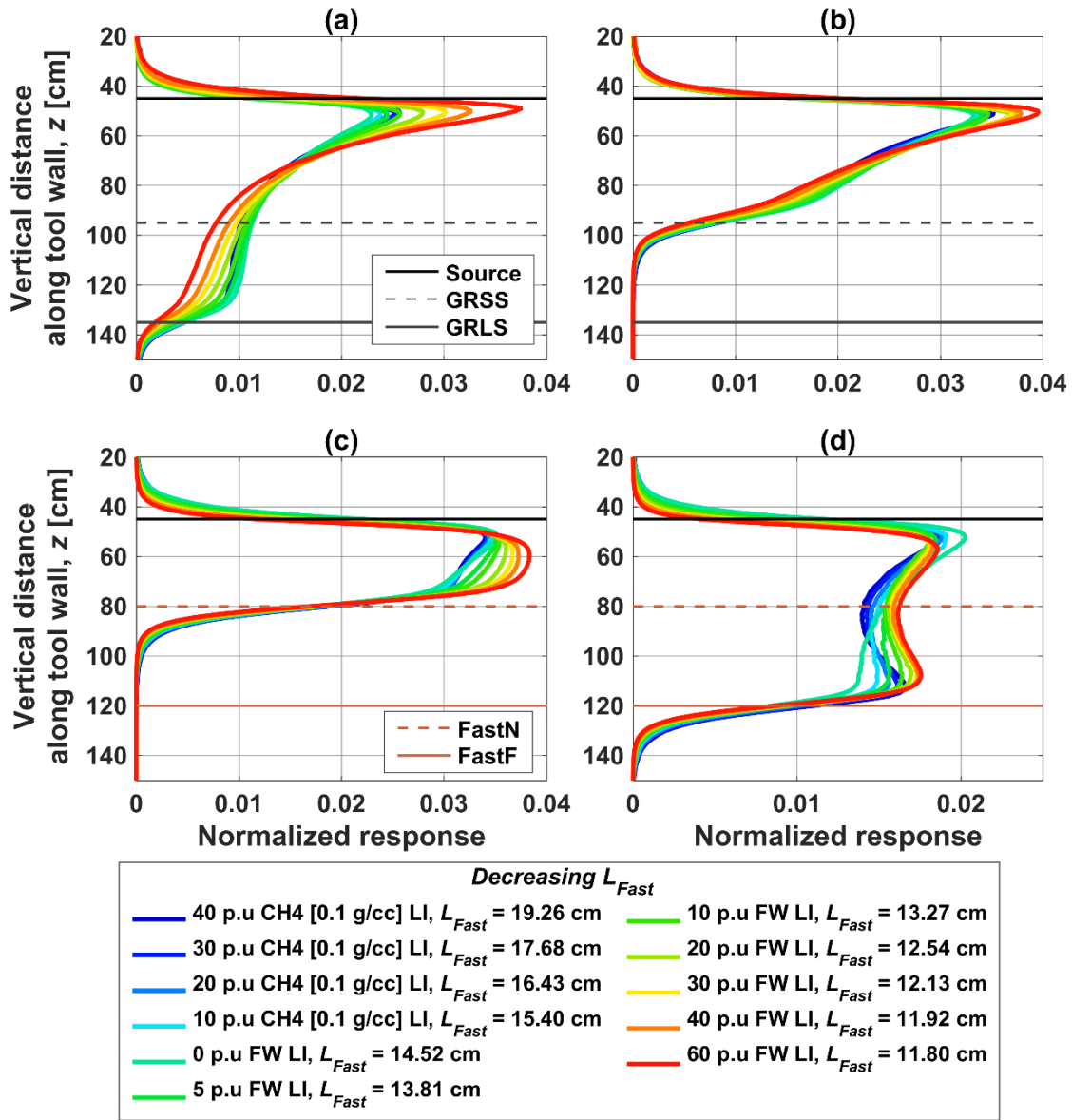


Figure 3.4. Library of fast neutron sensitivity functions integrated in the radial and azimuthal directions at (a) long- and (b) short-spaced gamma-ray detectors, (c) near and (d) far fast neutron detectors. The transition from blue to red denotes a decrease in fast slowing-down length, L_{Fast} . Solid black line at 45 cm (18 in) indicates the position of the pulsed neutron source, and the grey lines at 95 cm (37 in, solid line) and 135 cm (53 in, dashed line) indicate the location of short-, and long-spaced gamma-ray detectors, respectively. The locations of the near and far fast neutron detectors at 80 and 120 cm (31 and 47 in) are identified by dashed and solid brown lines, respectively.

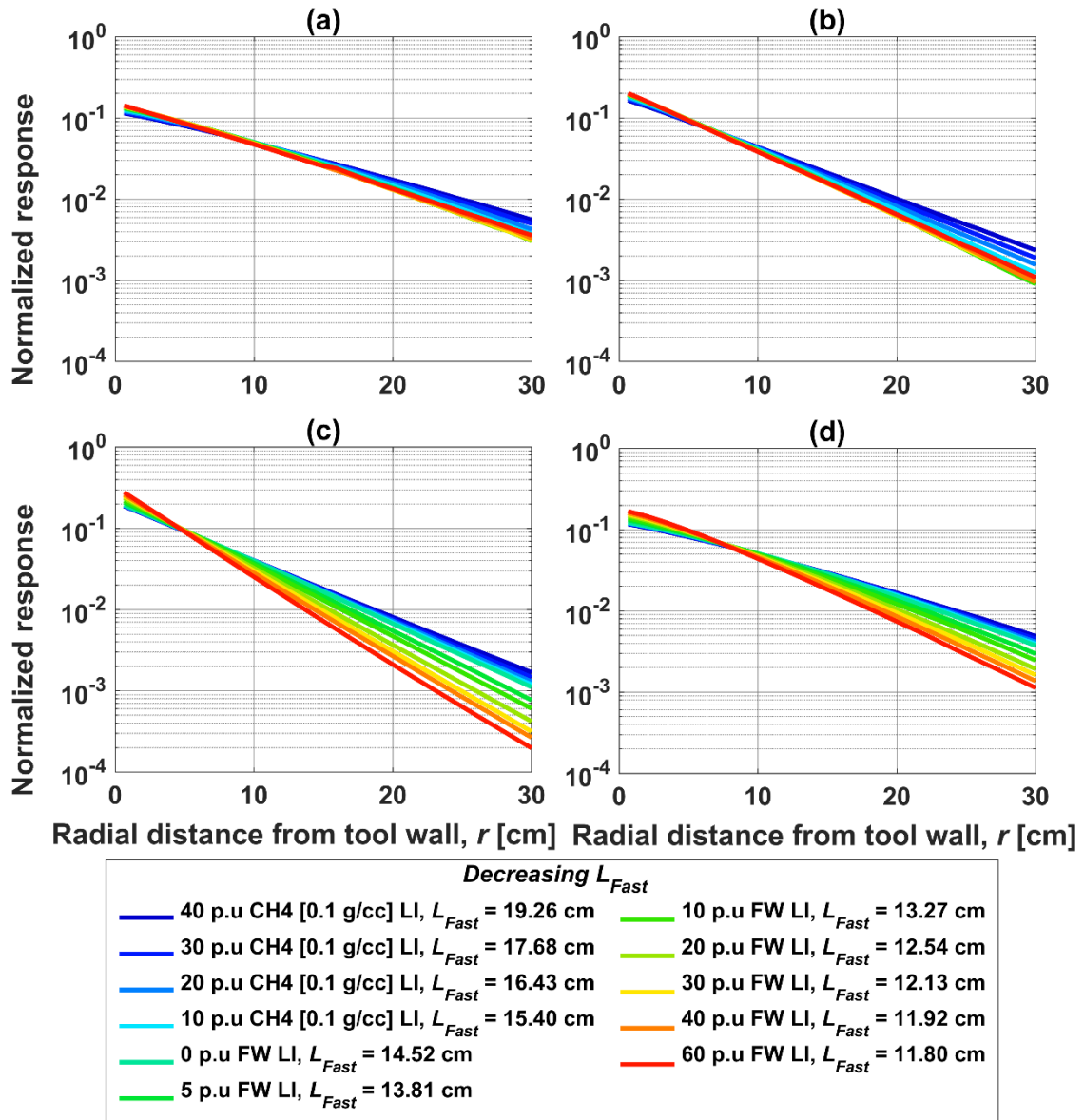


Figure 3.5. Library of fast neutron sensitivity functions integrated in the vertical and azimuthal directions at the (a) long- and (b) short-spaced gamma-ray detectors, (c) near and (d) far fast neutron detectors. The transition from blue to red denotes a decrease in fast slowing-down length, L_{Fast} .

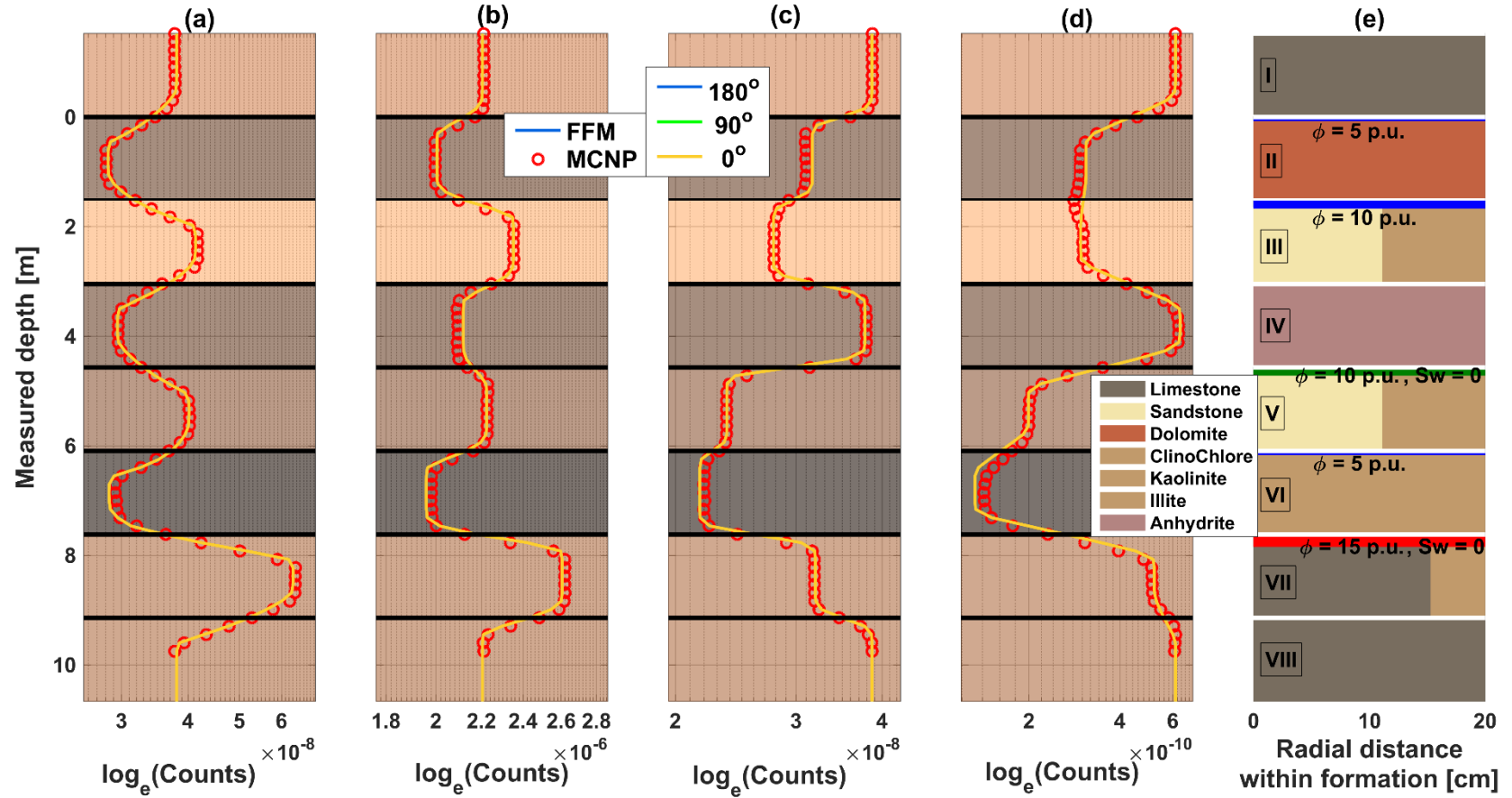


Figure 3.6. Synthetic Case 1 - Detector counts obtained with Monte Carlo simulations (red circles) at the bottom-sector (180°), and simulated with the fast-forward algorithm (solid lines) for a vertical well penetrating a sequence of 1.52-m (true stratigraphic thickness, TST) layers exhibiting complex mineralogy at (a) long- and (b) short-spaced gamma-ray detectors, (c) near and (d) far fast neutron detectors; (e) volumetric rock composition of the layered earth model (**Table 3.2**).

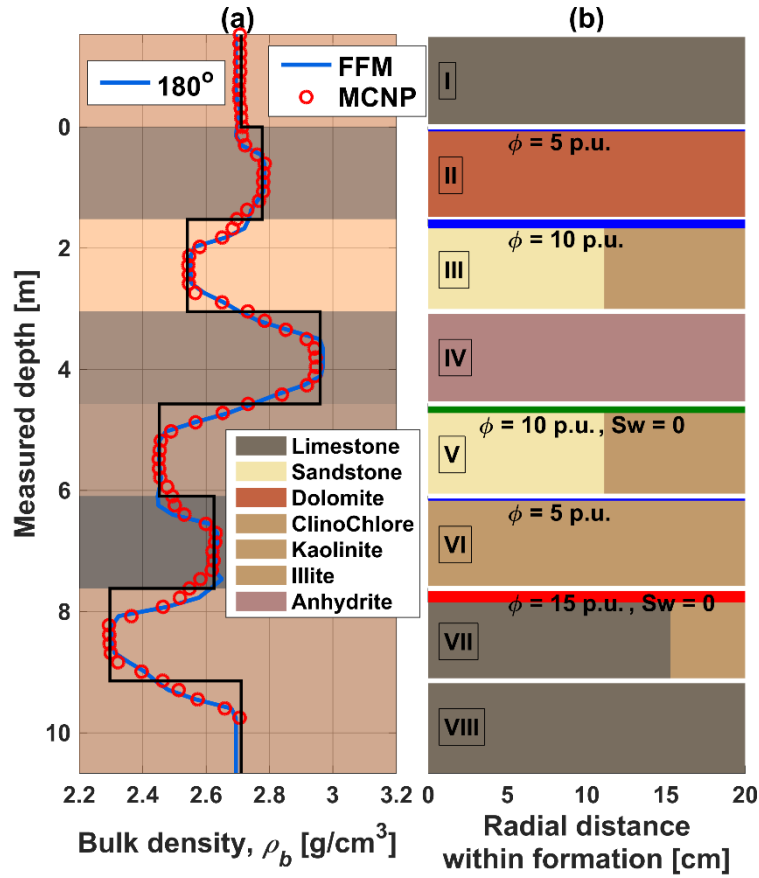


Figure 3.7. Synthetic Case 1 - (a) Bulk density, ρ_b , calculated from bottom-sector Monte Carlo (red circles) and fast-forward (blue solid line) detector counts for a vertical well penetrating a sequence of 1.52-m (true stratigraphic thickness, TST) layers exhibiting complex mineralogy. The blocky black line identifies bulk density for each bed. (b) Volumetric rock composition of the layered earth model (**Table 3.2**).

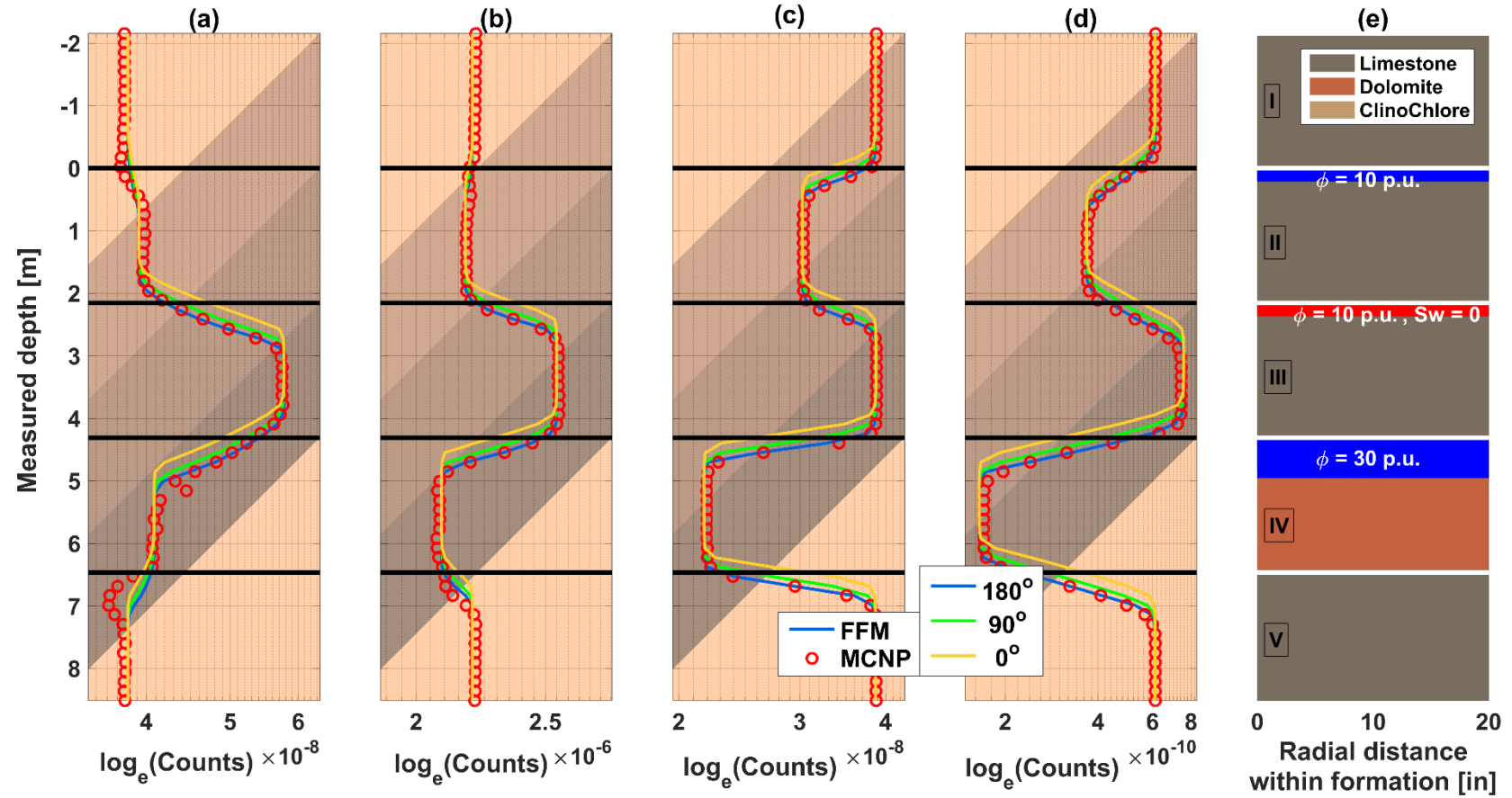


Figure 3.8. Synthetic Case 2 - Detector counts obtained with Monte Carlo simulations (red circles) at the bottom-sector (180°), and with the fast-forward algorithm (solid lines) for a 45° deviated well penetrating a sequence of 1.52-m (true stratigraphic thickness, TST) layers at (a) long- and (b) short-spaced gamma-ray detectors, (c) near and (d) far fast neutron detectors; (e) volumetric rock composition of the layered earth model (**Table 3.3**).

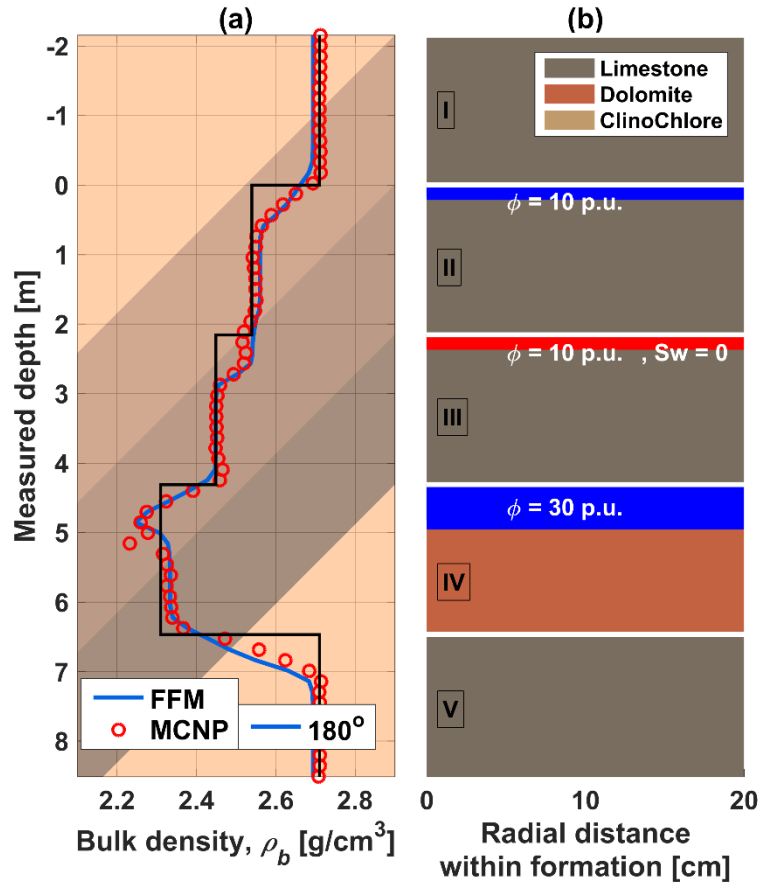


Figure 3.9. Synthetic Case 2 - (a) Bulk density, ρ_b , calculated from bottom-sector Monte Carlo (red circles) and fast-forward (blue solid line) detector counts for a 45° deviated well penetrating a sequence of 1.52-m (true stratigraphic thickness, TST) layers. The blocky black line identifies bulk density for each bed. (b) Volumetric rock composition of the layered earth model (**Table 3.3**).

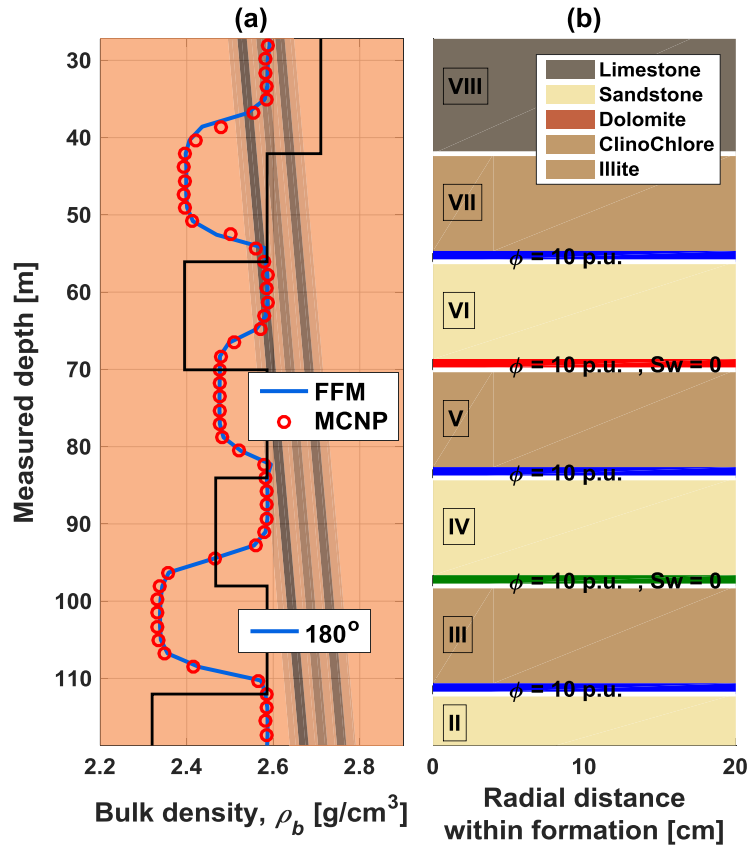


Figure 3.10. Synthetic Case 3 - (a) Bulk density, ρ_b , calculated from bottom-sector Monte Carlo (red circles) and fast-forward (blue solid line) detector counts for an 85° deviated well penetrating a sequence of 1.52-m (true stratigraphic thickness, TST) layers filled with freshwater, oil, and gas. The blocky black line identifies bulk density for each bed. (b) Volumetric rock composition of the layered earth model (**Table 3.4**).

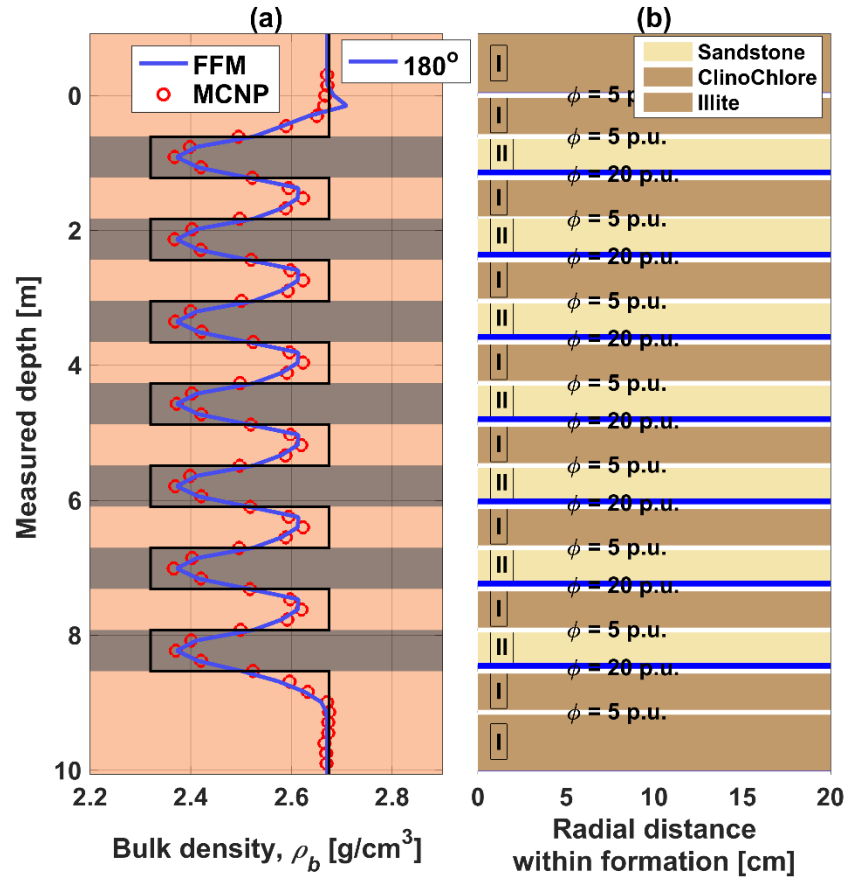


Figure 3.11. Synthetic Case 4A - (a) Bulk density, ρ_b , calculated from bottom-sector Monte Carlo (red circles) and fast-forward (blue solid line) detector counts for a vertical well penetrating a sequence of 61-cm (true stratigraphic thickness, TST) layers. The blocky black line identifies bulk density for each bed. (b) Volumetric rock composition of the layered earth model (**Table 3.5**).

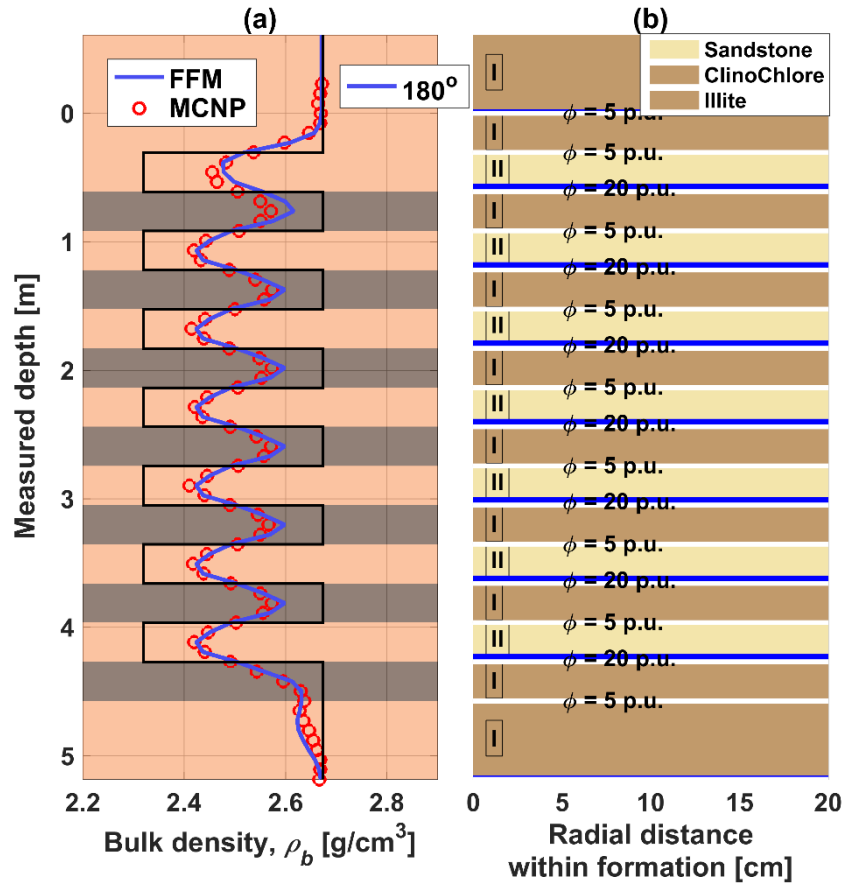


Figure 3.12. Synthetic Case 4B - (a) Bulk density, ρ_b , calculated from bottom-sector Monte Carlo (red circles) and fast-forward (blue solid line) detector counts for a vertical well penetrating a sequence of 30.5-cm (true stratigraphic thickness, TST) layers. The blocky black line identifies bulk density for each bed. (b) Volumetric rock composition of the layered earth model (**Table 3.5**).

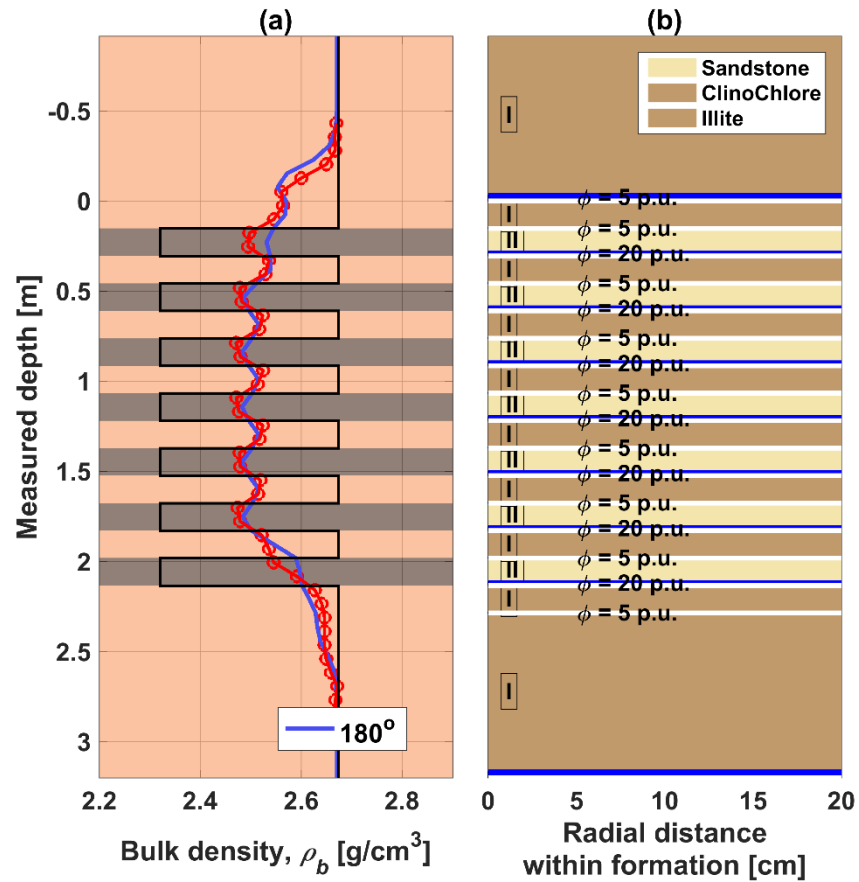


Figure 3.13. Synthetic Case 4C - (a) Bulk density, ρ_b , calculated from bottom-sector Monte Carlo (red circles) and fast-forward (blue solid line) detector counts for a vertical well penetrating a sequence of 15-cm (true stratigraphic thickness, TST) layers. The blocky black line identifies bulk density for each bed. (b) Volumetric rock composition of the layered earth model (**Table 3.5**).

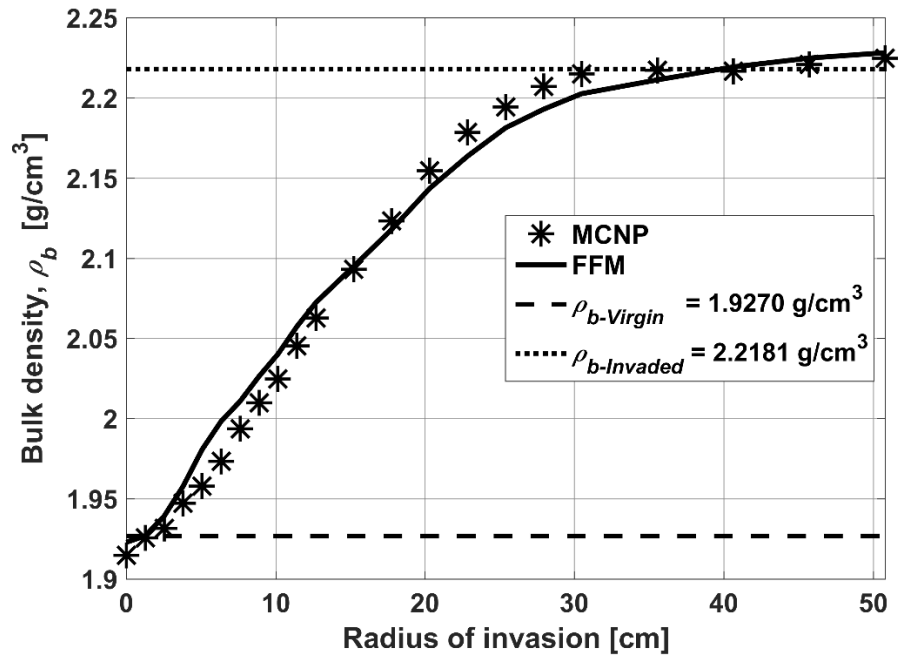


Figure 3.14. Synthetic Case 5 - Comparison of bulk density, ρ_b , simulated with the Monte Carlo and fast-forward methods with 100 kppm NaCl brine invading a 30-p.u. gas-bearing (0.1 g/cm³ CH₄) limestone formation (piston-like invasion).

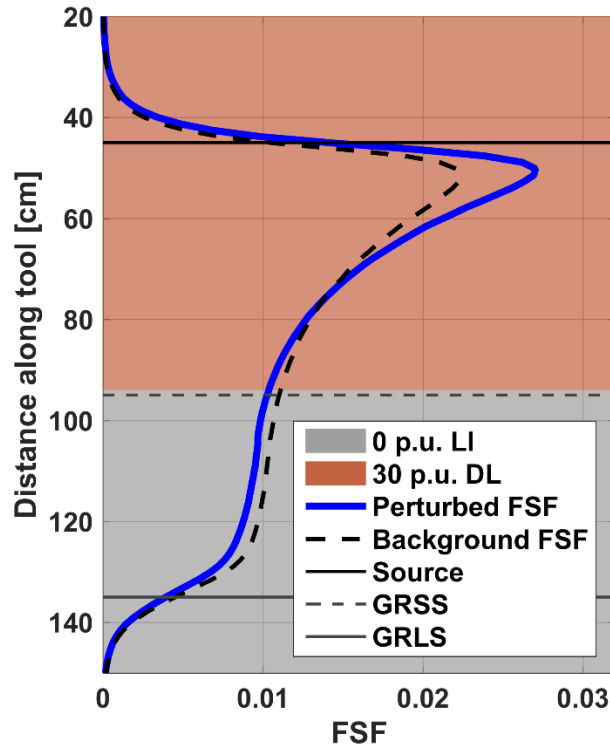


Figure 3.15. Comparison of sensitivity functions integrated in the radial and azimuthal directions acquired at the long-spaced gamma-ray detector. Solid blue line identifies MC-generated FSF for the layered formation and dashed black line is background sensitivity function for a homogeneous formation. Solid black line at 45 cm (18 in) indicates the position of the pulsed neutron source, and the grey lines at 95 cm (37 in, solid line) and 135 cm (53 in, dashed line) indicate the location of short-, and long-spaced gamma-ray detectors, respectively.

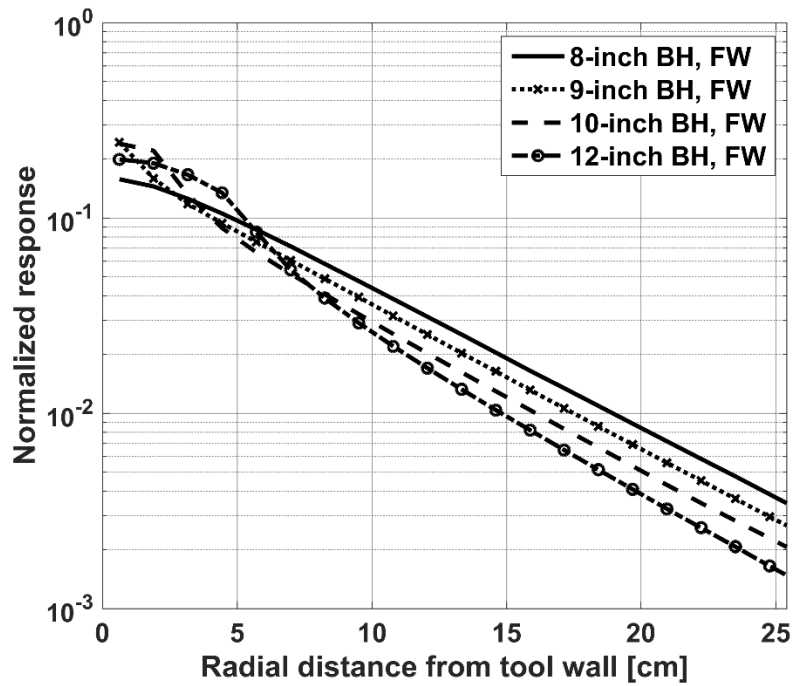


Figure 3.16. Comparison of MC sensitivity functions integrated in the vertical and azimuthal directions at the long-spaced gamma-ray detector, computed for 20.3-cm (8-in), 22.9-cm (9-in), 25.4-cm (10-in), and 30.5-cm (12-in) freshwater-filled boreholes. Tool diameter is 20.3 cm (8 in) and the formation is a 0 p.u. limestone block.

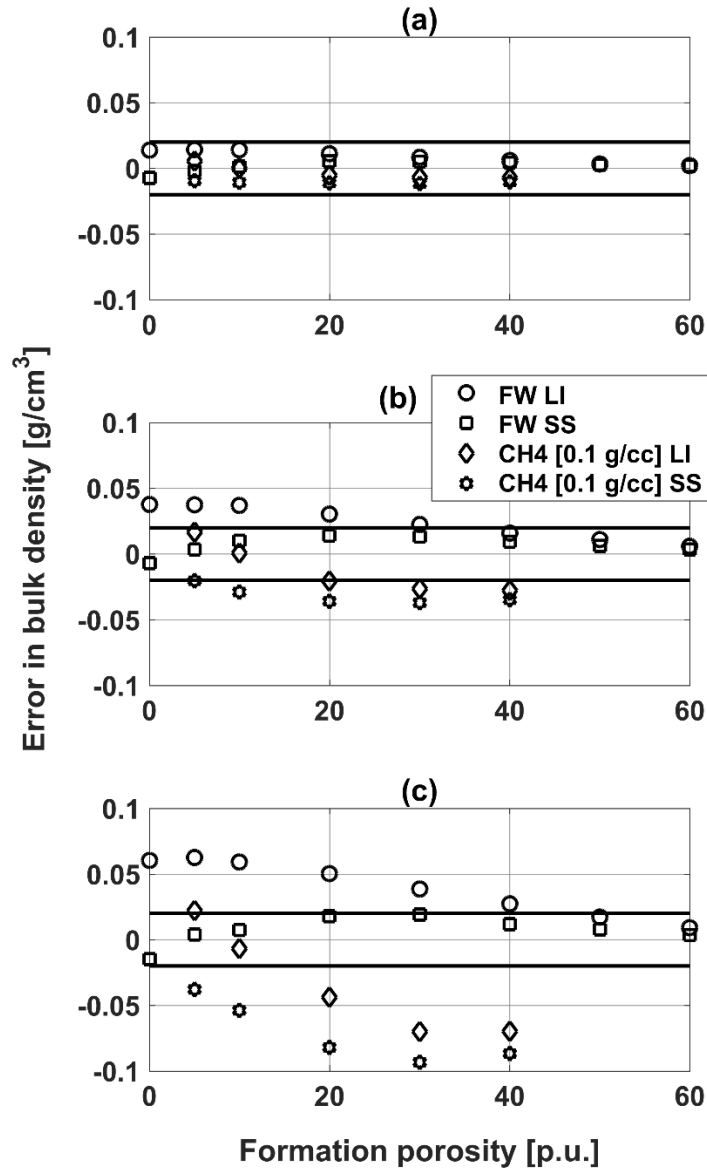


Figure 3.17. Difference between FF and MC-derived bulk densities in 22.9-cm (9-in), 25.4-cm (10-in), and 30.5-cm (12-in) freshwater-filled boreholes across freshwater and gas-filled (0.1 g/cm^3 CH₄) limestone (LI) and sandstone (SS) formations. Solid black lines identify $\pm 0.02 \text{ g/cm}^3$, respectively.

Chapter 4: Improvements of Fast Modeling of LWD Neutron Logs in Enlarged Boreholes for a Commercial LWD Tool

In complex geological environments, interpretation methods based on fast modeling and inversion procedures deliver better estimates of petrophysical properties than conventional methods. Neutron measurements are affected by higher-order formation and borehole effects. Their depth of investigation is also very sensitive to porosity, borehole size variations, and fluid and rock properties. Consequently, reliable petrophysical interpretation of neutron logs under complex rock and geometrical conditions requires fast modeling methods.

I develop a fast-forward algorithm for a commercial LWD neutron tool. The algorithm is based on perturbation theory, flux sensitivity functions (FSFs), and diffusion flux-difference (DFD) approximations. The DFD method interpolates between Monte Carlo (MC)-derived, base-case FSFs using one-group diffusion models and a Rytov approximation. Diffusion approximations successfully capture sensitivity flux perturbations: neutron porosities simulated using DFD-perturbed and MC-derived FSFs agree within 1 porosity unit (p.u.) in highly deviated wells, in enlarged boreholes, and with invasion. They significantly outperform linear interpolation approaches, improving accuracy by as much as 10 p.u.

Even when diffusion approximations are applied, perturbation theory may still yield inaccurate results when compared to neutron porosity estimated from MCNP counts for regions exhibiting contrasting properties, and primarily enlarged boreholes. I introduce a new two-step algorithm to improve neutron modeling accuracy to MCNP counts in the presence of standoff. The algorithm is based on

two sets of base cases: one for detector counts, and the other for sensitivity functions. On one hand, diffusion flux-difference approximations are used to compute perturbed sensitivity functions for any tool, borehole, and formation configuration. On the other hand, count base cases obtained for 21.6-cm (8.5-in), 24.1-cm (9.5-in), and 26.7-cm (10.5-in) boreholes extend the validity of the Taylor series expansion by minimizing the size of the borehole perturbations.

Compared to neutron porosity calculated from MCNP counts, the new algorithm yields relatively low errors in enlarged boreholes. Comparison benchmarks against synthetic cases confirmed good agreement with Monte Carlo simulations. Vertical and high-angle wells were assumed with the tool penetrating several bed layers with contrasting hydrogen index. Monte Carlo simulations were carried out to simulate neutron detector counts and to compare against results obtained from the proposed fast-forward algorithm.

4.1 INTRODUCTION

Conventional interpretation methods improperly estimate petrophysical properties in high-angle wells, in the presence of invasion, borehole effects, or for thinly-bedded formations. For nuclear measurements, procedures based on fast modeling and inversion were developed to overcome these limitations.

Borehole nuclear measurements are traditionally simulated using Monte-Carlo (MC) algorithms such as MCNP (Monte-Carlo N-Particle code, Goorley, 2014). Although flexible and accurate, such codes are computationally expensive, thus impractical for implementation with inverse problems. Watson (1984, 1992) first introduced modeling methods based on perturbation theory and sensitivity

maps. Mendoza et al. (2007, 2010a, 2010b) showed that spatial flux sensitivity functions (FSFs) coupled with iterative linear interpolations (the linear iterative refinement algorithm) accurately simulate borehole nuclear measurements across diverse geological environments. In challenging environments presenting sharp contrasts in formation properties, advanced techniques were implemented to account for higher-order effects. They are based on second-order approximations for density measurements (Zhou et al., 2009), or diffusion flux-difference (DFD) calculations for neutron measurements (Ijase et al., 2013a). These algorithms are several folds faster than MCNP and encouraged the development of inversion-based workflows for the petrophysical interpretation of nuclear measurements (Mendoza et al., 2012; Heidari et al., 2012, 2013; Ijase et al., 2013b).

Ijase et al. (2013a) showed that diffusion approximations accurately quantify flux perturbations: neutron porosities calculated using MC-derived and DFD-perturbed sensitivity functions agree within 1 porosity unit. However, their work did not include benchmarking against neutron porosity calculated from MCNP detector counts. When compared to neutron porosity derived from detector counts, the diffusion flux-difference algorithm has low accuracy in enlarged boreholes.

Coupled with the diffusion flux-difference method, I introduce a new two-step algorithm to accurately simulate borehole environmental effects in neutron measurements. Using several count base cases, in addition to sensitivity function base cases, I minimize the size of the borehole perturbations, thus improving accuracy. This new algorithm was implemented and tested with a commercial LWD neutron tool from Baker Hughes, a GE company. In homogeneous formations with standoff, and in synthetic examples, simulated neutron porosity yields an accuracy

of 0.9 p.u. on average, when compared to neutron porosity calculated from MCNP detector counts.

4.2 METHOD

4.2.1 Background Information on Tool Design

The algorithm was tested with a logging-while-drilling (LWD) commercial neutron tool (Baker Hughes 6 $\frac{3}{4}$ -inch CCNTM). It operates with an americium-beryllium (AmBe) neutron source. Its outer diameter is 19.8 cm (7.8 in), with a minimum borehole size of 21.6 cm (8.5 in). Baker Hughes provided MCNP modeling results including neutron counts and sensitivity maps at near and far detectors, for freshwater and gas-filled limestone, sandstone, and dolomite formations, in 21.6-cm (8.5-in), 24.1-cm (9.5-in), and 26.7-cm (10.5-in) boreholes.

4.2.2 Base-Cases Library

Fast-forward modeling algorithms based on perturbation theory simulate borehole nuclear measurements using a library of base-case FSFs precomputed in homogeneous formations (Mendoza et al., 2010a). **Table 4.1** lists the homogeneous rock compositions considered when simulating the base-case sensitivity functions, FSF_{b-FSF} , using MCNP. In addition to FSF base cases, count base cases are introduced to minimize the size of the borehole perturbations, thus increasing the validity of the Taylor series expansion. There are three count base cases at each neutron detector for borehole diameters equal to 21.6 cm (8.5 in), 24.1 cm (9.5 in), and 26.7 cm (10.5 in). **Figure 4.1** shows the calibration between MCNP detector counts for each base case and the inverse of formation migration length.

4.2.3 Detector Response Perturbation

The perturbed detector response $N(\mathbf{r}_R)$ at detector location $\mathbf{r}_R$ is expressed as (Ijasa et al., 2013a)

$$N(\mathbf{r}_R) \approx N_b(\mathbf{r}_R) + N_b(\mathbf{r}_R) \int d\mathbf{r} \text{FSF}_{DFD}(\mathbf{r}_R, \mathbf{r}) \frac{\Delta\alpha(\mathbf{r})}{\alpha_b}, \quad (4.1)$$

where N_b is background detector response, $\mathbf{r}$ is position vector in three-dimensional (3D) space, FSF_{DFD} is perturbed sensitivity function calculated using the diffusion flux-difference method, and α_b is modified cross section parameter associated with the homogeneous background formation. The difference $\Delta\alpha(\mathbf{r})$ represents the perturbation between the earth model, EM , described with modified cross section $\alpha_{EM}(\mathbf{r})$, and the homogeneous background formation, such that,

$$\Delta\alpha(\mathbf{r}) = \alpha_{EM}(\mathbf{r}) - \alpha_b. \quad (4.2)$$

4.2.4 Diffusion Flux-Difference (DFD) Method

Ijasa et al. (2013a) developed the diffusion flux-difference method to quantify sensitivity flux perturbations across layers exhibiting significant contrast in neutron cross section. Flux perturbations are predicted using a first-order Rytov approximation, such that,

$$\log_e \text{FSF}_{DFD}(\mathbf{r}_R, \mathbf{r}) - \log_e \text{FSF}_b(\mathbf{r}_R, \mathbf{r}) \approx \frac{\frac{d\psi_b(\mathbf{r})}{d\alpha_b}}{\psi_b(\mathbf{r})} \Delta\alpha(\mathbf{r}), \quad (4.3)$$

where FSF_b is background sensitivity function associated with the homogeneous background formation. The background analytical flux, ψ_b , and its derivative with respect to modified cross section α_b , $\frac{d\psi_b}{d\alpha_b}$, are computed from one-group neutron diffusion models (Ijasan et al., 2013a).

The diffusion model is corrected to account for higher-order transport effects using a modified neutron parameter α , which is given by,

$$\alpha = \frac{1}{L'_{1E}} = \frac{1}{\eta L_m}, \quad (4.4)$$

where L_m is migration length, L'_{1E} is modified migration length, and η is the transport-correction coefficient. Migration length is calculated using UTNuPRO (University of Texas – Nuclear Properties), an algorithm that implements a revised Kreft's method (Kreft, 1974), and yields migration length estimates in milliseconds and within 2.5% accuracy as compared to MCNP. **Figure 4.2** shows a cross-plot between modified migration length and migration length for the Baker LWD neutron tool.

4.2.5 New Two-Step Algorithm for Rapid Simulations of Neutron Measurements in Enlarged Boreholes

I introduce a new algorithm to improve the accuracy of simulated neutron measurements in enlarged boreholes. Using two different sets of base cases, one for detector counts, and the other for sensitivity functions, borehole perturbations are minimized in a least-square sense, thus improving the accuracy of the fast-forward algorithm.

On one hand, count base cases, $b-C$, are computed in formations associated with modified cross section $\alpha_{b-C}(\mathbf{r})$ for three boreholes with diameters of 21.6 cm (8.5 in), 24.1 cm (9.5 in), and 26.7 cm (10.5 in). Parameter $\alpha_{b-C}(\mathbf{r})$ is defined such that

$$\alpha_{b-C}(\mathbf{r}) = \begin{cases} \alpha_{b-C}^{Borehole} & , \mathbf{r} \in Borehole \\ \alpha_{b-C}^{Formation}(\mathbf{r}) & , \mathbf{r} \in Formation \end{cases}, \quad (4.5)$$

where $\alpha_{b-C}^{Borehole}$ and $\alpha_{b-C}^{Formation}(\mathbf{r})$ are the modified cross sections associated with the count base cases of the borehole and the formation, respectively.

On the other hand, MC-derived FSF base cases, $b-FSF$, are computed for a 21.6-cm (8.5-in) borehole in homogeneous formations associated with modified cross section α_{b-FSF} (**Table 4.1**). In enlarged boreholes, perturbed sensitivity function, FSF_{DFD} , is calculated using the diffusion flux-difference method (Ijisan et al., 2013a), such that

$$FSF_{DFD}(\mathbf{r}_R, \mathbf{r}) \approx FSF_{b-FSF}(\mathbf{r}_R, \mathbf{r}) \cdot \exp \left\{ \left[\alpha_{EM}(\mathbf{r}) - \alpha_{b-FSF} \right] \cdot \frac{d\psi_{b-FSF}(\mathbf{r})}{d\alpha_{b-FSF}} / \psi_{b-FSF}(\mathbf{r}) \right\}, \quad (4.6)$$

In equation 4.6, the earth model is described by modified cross section $\alpha_{EM}(\mathbf{r})$, given by

$$\alpha_{EM}(\mathbf{r}) = \begin{cases} \alpha_{EM}^{Borehole} & , \mathbf{r} \in Borehole \\ \alpha_{EM}^{Formation}(\mathbf{r}) & , \mathbf{r} \in Formation \end{cases}, \quad (4.7)$$

where $\alpha_{EM}^{Borehole}$ and $\alpha_{EM}^{Formation}(\mathbf{r})$ are the modified cross sections associated with the earth model for the borehole and the formation, respectively.

Figure 4.3 qualitatively compares MC-derived and DFD-perturbed sensitivity functions in homogeneous limestone formations. The diffusion flux-difference method successfully quantifies sensitivity flux variations for homogeneous perturbations smaller than 10 porosity units. On a Linux® cluster with Intel® Xeon® 6-core 2.9 GHz processors, MCNP calculations required approximately 300 minutes CPU-time for each case, whereas DFD-perturbed sensitivity functions were computed in 0.18 seconds on a Windows® PC, with an Intel® Core™ i7-7700HQ (2.80-GHz) processor. **Figure 4.4** qualitatively compares MC-derived and DFD-perturbed sensitivity functions with a 2.54-cm (1-in) standoff. DFD-perturbed sensitivity function, FSF_{DFD} , was computed in a 20 p.u. freshwater-filled limestone formation for a 26.7-cm (10.5-in) borehole filled with freshwater mud. Flux perturbations arising in the presence of standoff are accurately captured by DFD-perturbed sensitivity functions in radial (panels (c) and (g)), and vertical (panels (d) and (h)) directions. In contrast, sensitivity functions calculated using the linear iterative refinement method do not match MC-derived FSFs. The diffusion flux-difference method accurately quantifies flux perturbations with errors of 1 p.u. (Ijasa et al., 2013a). However, when compared to neutron porosity calculated using MCNP detector counts, diffusion flux-difference approximations yield inaccurate results in the presence of standoff.

I introduce a two-step process to accurately simulate neutron measurements in enlarged boreholes by minimizing the size of the perturbation such that $\Delta\alpha(\mathbf{r}) \ll \alpha_b$. With this condition, the approximation given by the Taylor series expansion (equation 4.1) becomes more accurate. The first step of the

algorithm uses the DFD-perturbed sensitivity function, FSF_{DFD} , to compute the perturbations from the formation as follows:

$$\alpha_{EM-eff}^{Formation} = \int d\mathbf{r} \frac{FSF_{DFD}(\mathbf{r}_R, \mathbf{r} \in \text{Formation})}{\int d\mathbf{r} FSF_{DFD}(\mathbf{r}_R, \mathbf{r} \in \text{Formation})} \cdot \alpha_{EM}^{Formation}(\mathbf{r}) , \quad (4.8)$$

where $\alpha_{EM-eff}^{Formation}$, the effective modified cross section of the formation, represents the impact of formation perturbations on the detector response. In the second step, an updated earth model, $\alpha_{EM-updated}(\mathbf{r})$ is defined by

$$\alpha_{EM-updated}(\mathbf{r}) = \begin{cases} \alpha_{EM-eff}^{Formation} + \alpha_{EM}^{Borehole} - \alpha_{b-C}^{Borehole} & , \mathbf{r} \in \text{Borehole} \\ \alpha_{EM-eff}^{Formation} & , \mathbf{r} \in \text{Formation} \end{cases} , \quad (4.9)$$

where $\alpha_{EM}^{Borehole} - \alpha_{b-C}^{Borehole}$ is the borehole perturbation. Then, perturbed detector response, N , is derived from equation 4.1, and given by

$$N(\mathbf{r}_R) \approx N_{b-C}(\mathbf{r}_R) + N_{b-C}(\mathbf{r}_R) \int d\mathbf{r} FSF_{DFD}(\mathbf{r}_R, \mathbf{r}) \cdot \frac{[\alpha_{EM-updated}(\mathbf{r}) - \alpha_{b-C}]}{\alpha_{b-C}} . \quad (4.10)$$

The flow diagram describing the DFD two-step fast-forward algorithm is shown in **Figure 4.5**.

4.3 BENCHMARK RESULTS

The DFD two-step algorithm was primarily developed to improve the accuracy of simulated neutron measurements in the presence of standoff. Therefore, benchmark cases include enlarged borehole configurations with up to 2.54-cm (1-in) standoff. Additionally, the algorithm was tested with two synthetic examples.

4.3.1 Borehole Environmental Effects

The diffusion flux-difference two-step algorithm was benchmarked in 21.6-cm (8.5-in), 24.1-cm (9.5-in), and 26.7-cm (10.5-in) boreholes, with freshwater and 30 kppm NaCl mud, across freshwater and gas-filled limestone, sandstone, and dolomite formations. In **Figure 4.6**, the maximum difference between neutron porosity directly estimated from MCNP counts, ϕ_{N-MC} , and porosity calculated using the DFD two-step algorithm, $\phi_{N-FSF_{DFD}}$, is 1.9 p.u. and root-mean-square error (RMSE) is 0.4 p.u. For 22.9-cm (9-in) and 25.4-cm (10-in) borehole diameters that were not included as part of the count base cases, the root-mean-square error is 0.9 p.u., while maximum error is 2 p.u. for freshwater mud, across freshwater-filled limestone and sandstone formations, up to 40 p.u. (**Figure 4.7**).

4.3.2 Synthetic Examples

The DFD two-step algorithm is also benchmarked using two synthetic examples featuring one vertical well and one high-angle/horizontal well. **Table 4.2** lists the layer properties assumed for Synthetic Case 1, including rock composition, true-stratigraphic-thicknesses (TST), migration length, bulk density, and hydrogen index (HI). Note that this synthetic case features a vertical well penetrating layers with contrasting hydrogen index and that the TST of several layers is below the

vertical resolution of the measurement (which is 49 cm or 19 in). **Figure 4.8** compares neutron porosity logs simulated with MCNP, ϕ_{N-MC} , and with the DFD two-step algorithm, $\phi_{N-FSF_{DFD}}$. The DFD two-step algorithm achieves maximum errors of 1 p.u. and average root-mean-square error of 0.5 p.u. with respect to MC simulations. The second synthetic example, Synthetic Case 2, features an 80° deviated well with layer properties described in **Table 4.3**. In **Figure 4.9**, the red markers and solid blue line identify neutron porosity logs simulated using MCNP and the DFD two-step algorithm, respectively. For this synthetic example, the DFD two-step algorithm yields maximum errors of 2 p.u. and average root-mean-square errors of 0.6 p.u. compared to MCNP.

4.4 CONCLUSIONS

Inversion-based interpretation of neutron logs in enlarged boreholes is complex because neutron measurements are affected by higher-order effects in the form of sensitivity flux perturbations. Although diffusion flux-difference approximations can quantify such flux perturbations in spatially complex geometries, Taylor series approximations still produce non-negligible errors in the presence of standoff.

I introduce a new fast-forward modeling algorithm based on a two-step implementation process coupled with diffusion flux-difference approximations. On one hand, perturbed sensitivity functions are computed with the DFD method for any borehole size, orientation, and eccentricity using nine precalculated base-case FSFs. On the other hand, the effect of formation and borehole perturbations are simulated separately, in two steps, with respect to pre-computed count base

cases. This method accurately simulates neutron measurements in the presence of standoff because it minimizes the size of the borehole perturbations, thus improving the estimations given by the Taylor series expansion.

Simulated neutron porosities were benchmarked against neutron porosities calculated with MCNP detector counts. The DFD two-step algorithm yields maximum errors of 2 p.u. and root-mean-square errors of 1 p.u. up to 2.54-cm (1-in) standoff.

Base Case	Volumetric Composition, [v/v]	Migration Length, L_m [cm]
FW LI - 0 p.u	0.00 H ₂ O, 1.00 CaCO ₃	28.0583
FW LI - 5 p.u	0.05 H ₂ O, 0.95 CaCO ₃	20.7965
CH ₄ [0.2 g/cm ³] LI - 30 p.u	0.30 CH ₄ , 0.70 CaCO ₃	18.6089
FW LI - 10 p.u	0.10 H ₂ O, 0.90 CaCO ₃	17.6751
FW LI - 20 p.u	0.20 H ₂ O, 0.80 CaCO ₃	14.2878
FW LI - 30 p.u	0.30 H ₂ O, 0.70 CaCO ₃	12.3431
FW LI - 40 p.u	0.40 H ₂ O, 0.60 CaCO ₃	11.0422
FW LI - 50 p.u	0.50 H ₂ O, 0.50 CaCO ₃	10.099
FW LI - 60 p.u	0.60 H ₂ O, 0.40 CaCO ₃	9.3791

Table 4.1. Homogeneous base case formations assumed for the calculation of neutron FSF_{b-FSF} in a 21.6-cm (8.5-in) borehole.

Layer	TST [ft]	Volumetric Composition [v/v]		Bulk Density [g/cm ³]	Migration Length [cm]	Hydrogen Index []
1	0.64	0.2 0.8	CH ₄ [0.176 g/cm ³] LI	2.2032	20.8326	0.0791
2	0.61	0.1 0.9	CH ₄ [0.176 g/cm ³] DL	2.6006	21.7856	0.0395
3	0.37	1	LI	2.7100	28.0583	0
4	0.46	0.05 0.95	CH _{1.78} [0.82 g/cm ³] LI	2.6155	20.9120	0.0381
5	0.52	1	LI	2.7100	28.0583	0
6	0.30	0.1 0.9	CH _{1.78} [0.82 g/cm ³] LI	2.6650	17.0912	0.0953
7	0.61	0.2 0.8	H ₂ O LI	2.3680	14.2878	0.2
8	0.55	0.1 0.9	H ₂ O LI	2.5390	17.6751	0.1

Table 4.2. Layer properties of the earth model corresponding to the synthetic case shown in **Figure 4.8**. TST stands for true-stratigraphic-thickness, LI for limestone, and DL for dolomite.

Layer	TST [ft]	Volumetric Composition [v/v]	Bulk Density [g/cm ³]	Migration Length [cm]	Hydrogen Index []
1	1.3	0.2 CH ₄ [0.176 g/cm ³] 0.8 SS	2.1552	23.3643	0.0791
2	1.2	0.1 CH _{1.78} [0.82 g/cm ³] 0.9 SS	2.4670	19.8800	0.0953
3	0.85	1 SS	2.65	34.6558	0
4	1.3	0.05 CH _{1.78} [0.82 g/cm ³] 0.95 SS	2.5585	24.0731	0.0476
5	1.2	1 SS	2.65	34.6558	0
6	1.5	0.2 H ₂ O 0.8 SS	2.3200	15.3955	0.2

Table 4.3. Layer properties of the earth model corresponding to Synthetic Case 2 featuring an 80° deviated well shown in **Figure 9**. TST stands for true-stratigraphic-thickness and SS for sandstone.

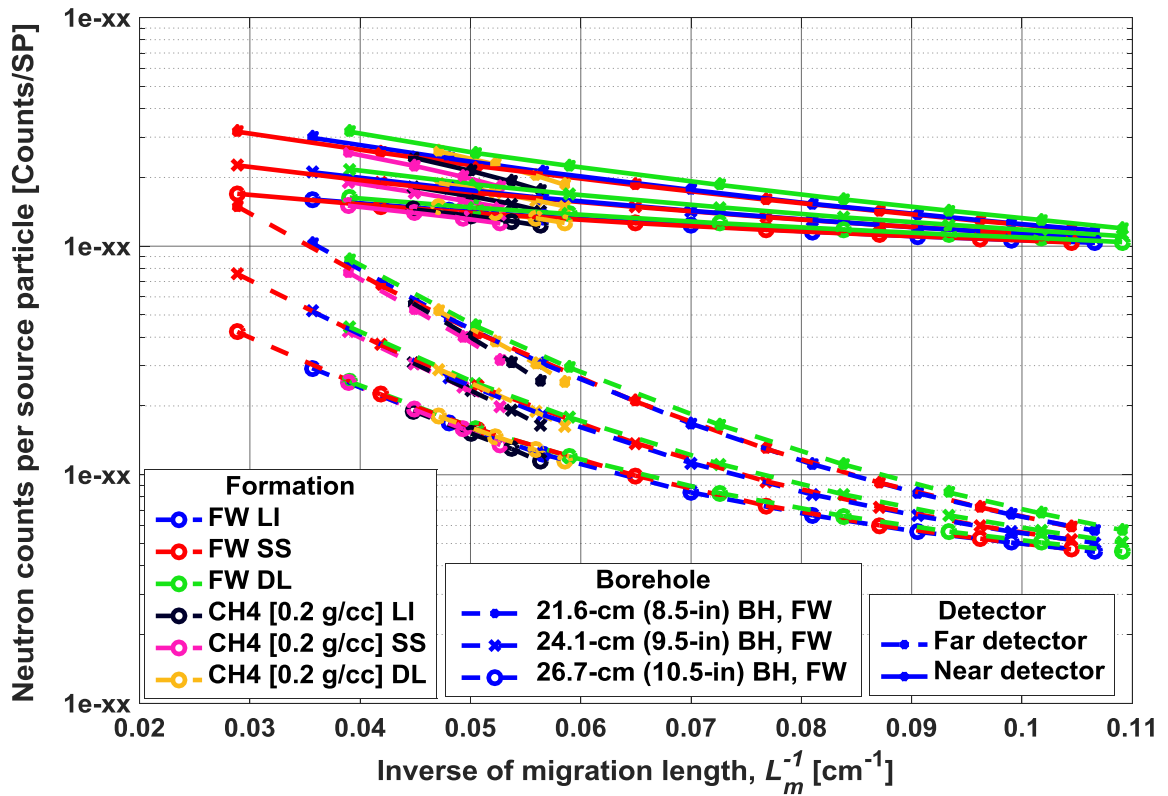


Figure 4.1: Cross-plot of neutron counts per source particle and the inverse of migration length at near and far detectors, for freshwater and gas-filled limestone, sandstone, and dolomite formations, in 21.6-cm (8.5-in), 24.1-cm (9.5-in), and 26.7-cm (10.5-in) boreholes. FW stands for freshwater, LI, for limestone, SS for sandstone, and DL for dolomite.

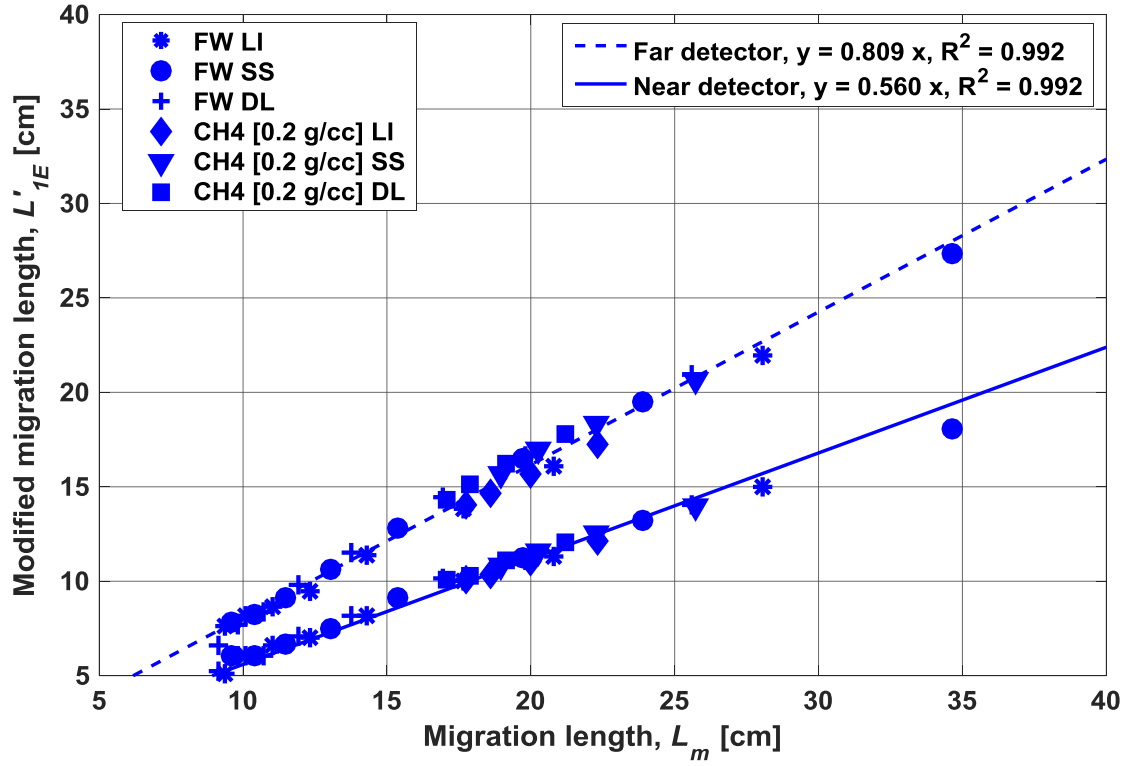


Figure 4.2. Cross-plot of modified travel length, L'_{1E} , and migration length, L_m , across freshwater and gas-filled sandstone, limestone, and dolomite formations. Slopes of dashed and solid lines identify corrections coefficients, η , for the far and near detectors, respectively. FW stands for freshwater, LI, for limestone, SS for sandstone, and DL for dolomite.

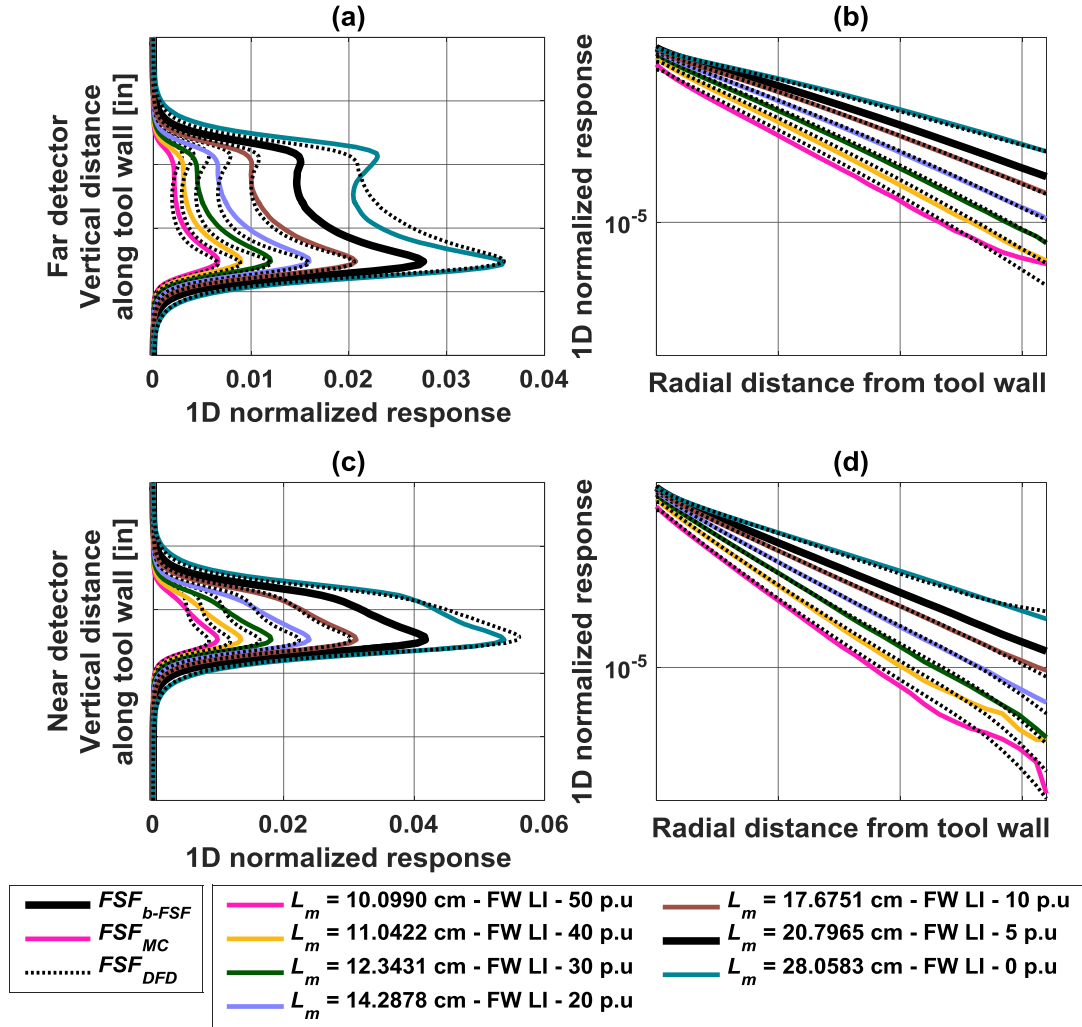


Figure 4.3. Qualitative comparison of MC-derived and perturbed diffusion flux-difference sensitivity functions in freshwater-filled limestone homogeneous formations. Left and right panels show sensitivity functions projected in vertical and radial directions, respectively. Top and bottom panels show sensitivity functions at far and near detectors, respectively. Solid lines identify MC-derived sensitivity functions, FSF_{MC} , with background sensitivity function, FSF_{b-FSF} , in black. Black dashed lines identify perturbed sensitivity functions, FSF_{DFD} , calculated from background FSF_{b-FSF} using the diffusion flux-difference method. (a) Sensitivity functions integrated in the azimuthal and radial directions at the far detector. (b) Sensitivity functions integrated in the azimuthal and vertical directions at the far detector. (c) Similar to (a) for the near detector. (d) Similar to (b) for the near detector. FW stands for freshwater, and LI, for limestone.

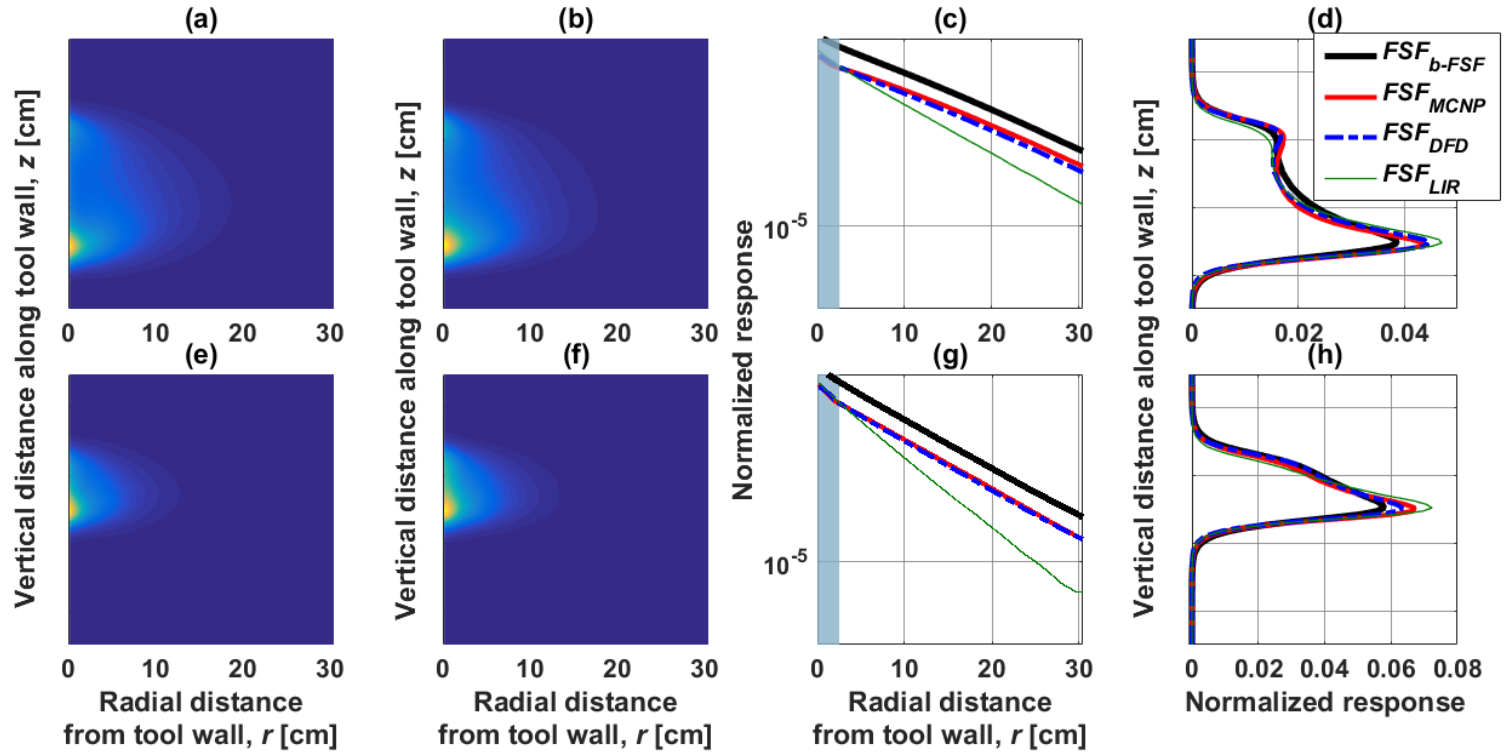


Figure 4.4. Qualitative comparison of MC-derived sensitivity function, FSF_{MC} , DFD perturbed sensitivity function, FSF_{DFD} , and sensitivity function calculated with the linear iterative refinement algorithm, FSF_{LIR} , for a 26.7-cm (10.5-in) borehole with freshwater mud, in a 20 p.u. freshwater-filled limestone formation. Top and bottom panels show sensitivity functions at far and near detectors, respectively. (a)(e) MC-derived sensitivity function integrated in the azimuthal direction. (b)(f) DFD perturbed sensitivity function integrated in the azimuthal direction. (c)(g) Sensitivity functions integrated in the vertical and azimuthal directions. MC-derived, DFD perturbed, LIR, and background sensitivity functions are identified by solid red, dashed blue, solid green, and solid black lines, respectively. (d)(h) Sensitivity functions integrated in the radial and azimuthal directions.

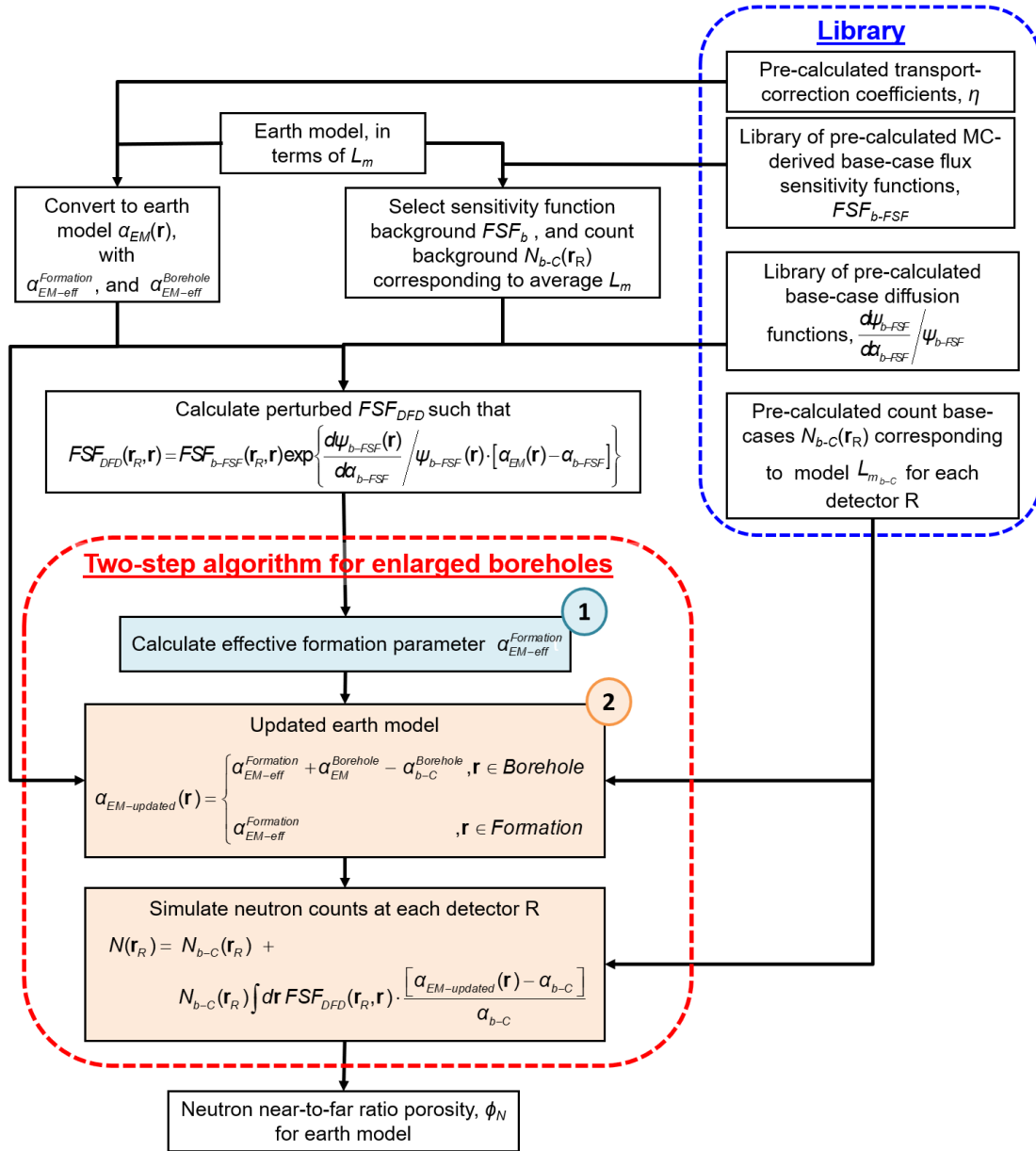


Figure 4.5. Flow diagram describing the implementation of the DFD method coupled with the two-step algorithm for enlarged boreholes. Dashed blue rounded rectangle identifies the library with the count and sensitivity function base cases, the transport correction coefficients, and the diffusion flux-difference functions. Dashed red rounded rectangle identifies the DFD two-step algorithm with the circles number 1 and 2 representing the first and second step, respectively.

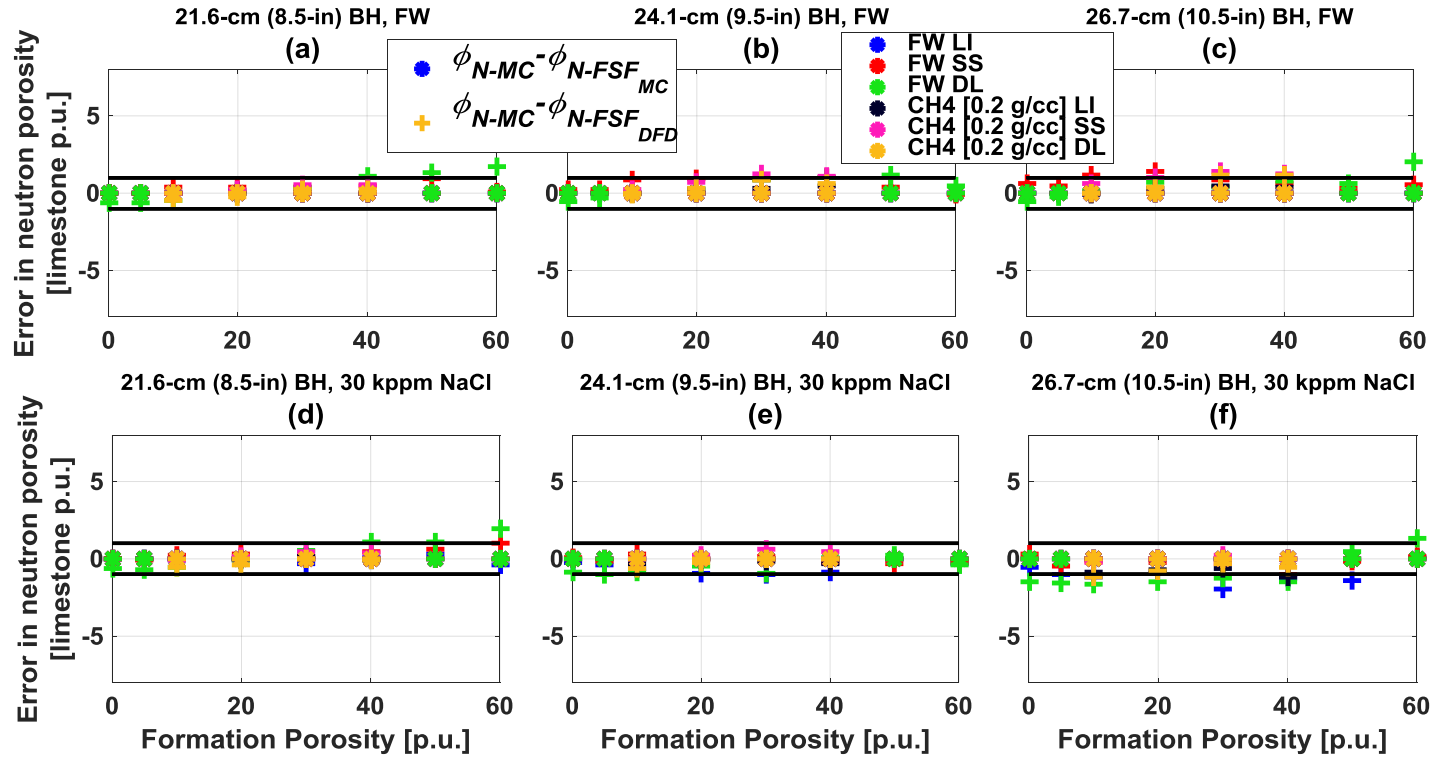


Figure 4.6. Quantitative comparison of neutron porosities calculated using MC-derived, $\phi_{N-FSF_{MC}}$, and DFD perturbed, $\phi_{N-FSF_{DFD}}$, sensitivity functions coupled with the two-step algorithm for enlarged boreholes, to neutron porosities directly estimated from MCNP counts, ϕ_{N-MC} , in freshwater and gas-filled limestone, sandstone, and dolomite formations. Comparisons are performed in (a)(c) 21.6-cm (8.5-in), (b)(d) 24.1-cm (9.5-in), and (c)(e) 26.7-cm (10.5-in) boreholes (centered tool configuration) with freshwater and 30 kppm NaCl mud. The solid black lines represent an error of 1 porosity unit. FW stands for freshwater, LI, for limestone, SS for sandstone, and DL for dolomite.

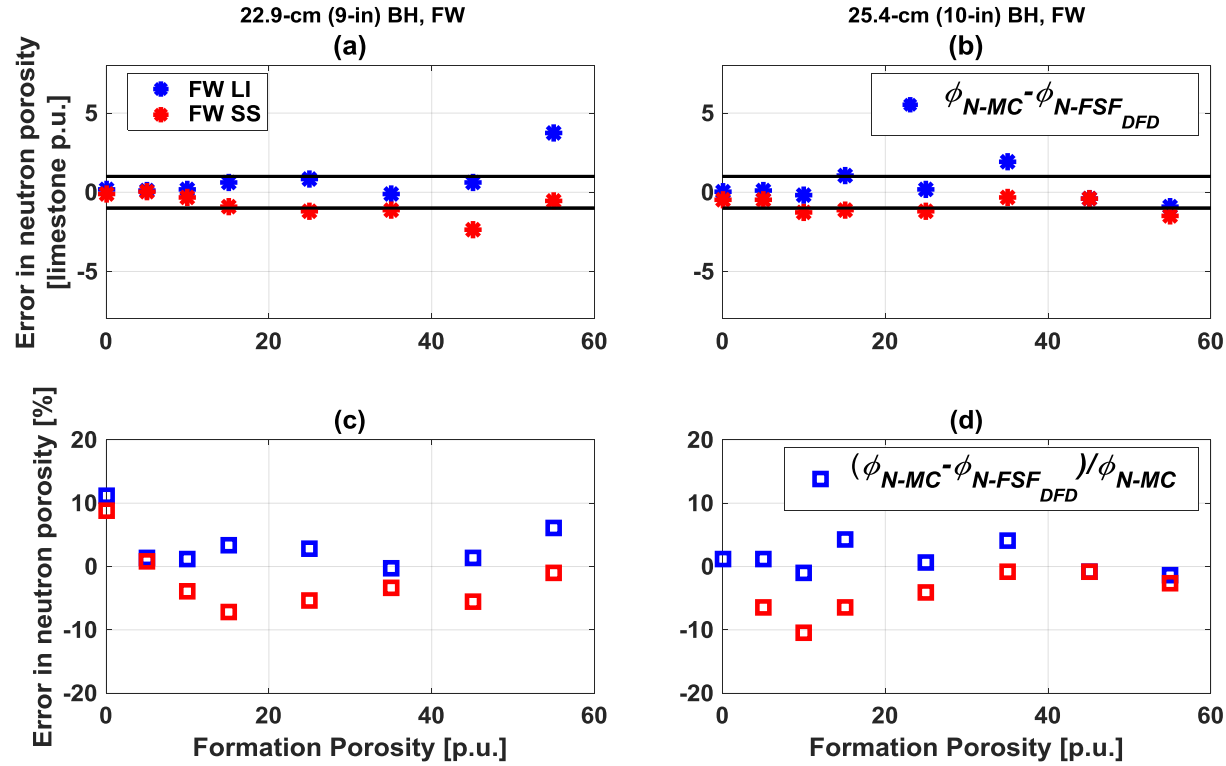


Figure 4.7. Quantitative comparison of neutron porosity calculated using DFD perturbed sensitivity functions coupled with the two-step algorithm for enlarged boreholes, $\phi_{N-FSF_{DFD}}$, and neutron porosity directly estimated from MCNP counts, ϕ_{N-MC} , in freshwater-filled limestone, and sandstone formations. Top panels show errors in limestone porosity units, and bottom panels, in percentage. Errors are computed for (a)(c) 22.9-cm (9-in), and (b)(d) 25.4-cm (10-in) boreholes (centered tool configuration) with freshwater mud. The solid black lines represent an error of 1 porosity unit. FW stands for freshwater, LI, for limestone, and SS for sandstone.

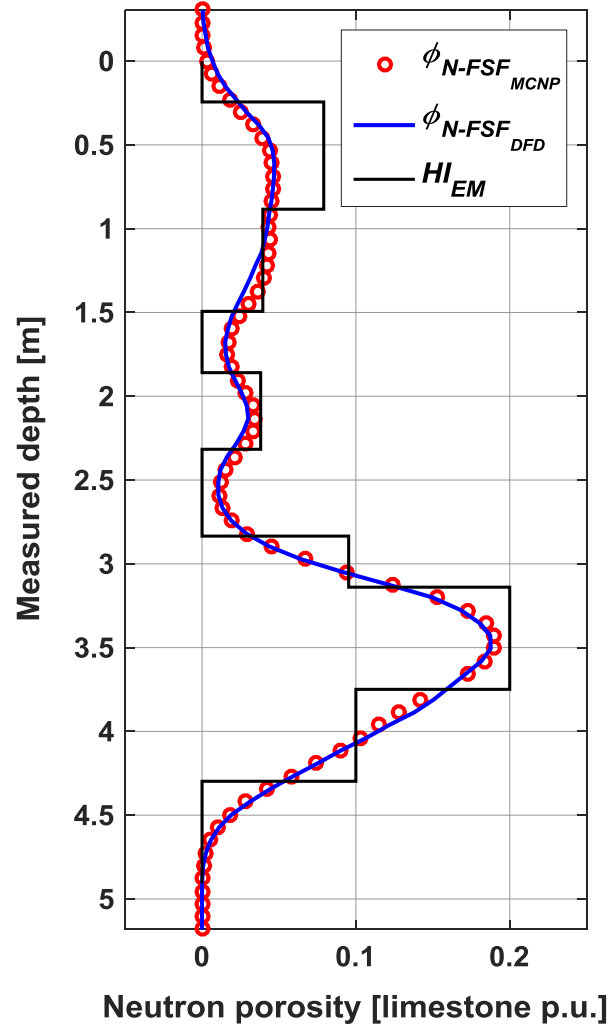


Figure 4.8. Comparison of LWD neutron porosity logs, ϕ_N , simulated with MCNP (red circles) and with the DFD two-step fast-forward algorithm (solid blue line). The blocky black line identifies the hydrogen index of the formation.

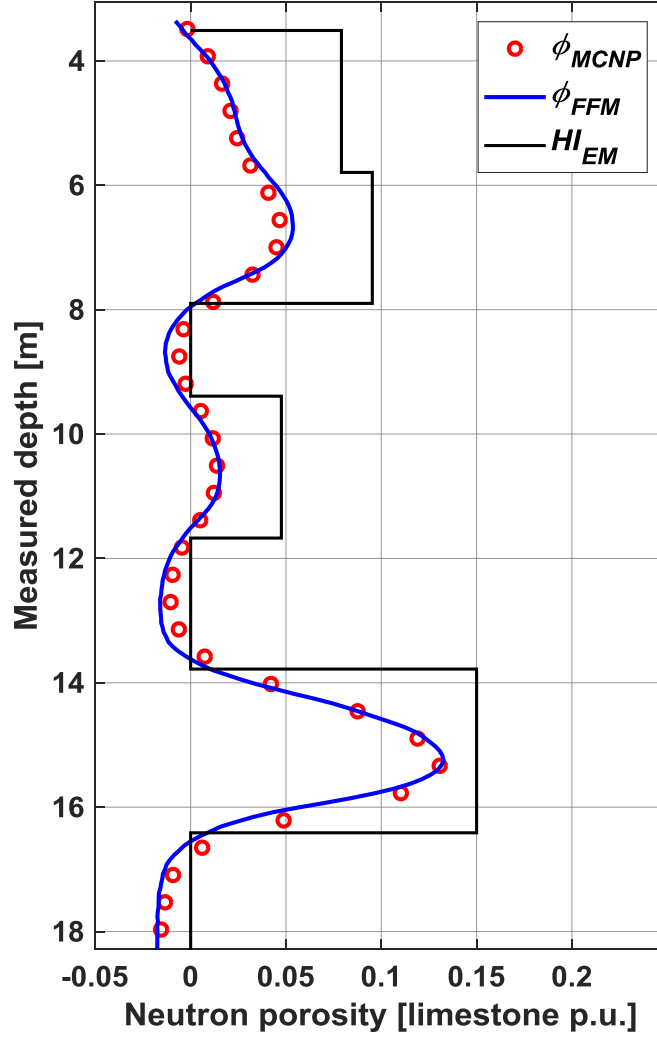


Figure 4.9. Comparison of LWD neutron porosity logs, ϕ_N , simulated with MCNP (red circles) and with the DFD two-step fast-forward algorithm (solid blue line) for Synthetic Case 2 which features an 80° deviated well. The blocky black line identifies the hydrogen index of the formation.

Chapter 5: Fast Modeling of Gamma-Gamma Density Measurements via Gamma-Ray Point Kernel Approximations

Forward modeling algorithms based on flux sensitivity functions (FSFs) are commonly recognized as fast, reliable, and the most efficient way to implement inversion-based interpretation algorithms for borehole nuclear measurements. Second-order sensitivity functions were developed to improve the accuracy of fast-forward modeling algorithms in complex geometries. However, their use is limited to Gamma-Gamma borehole density measurements.

I introduce an alternative method to second-order approximations in complex three-dimensional (3D) geometries. It is the first step toward future improvements to simulate borehole environmental effects, and to take into account arbitrary well trajectories for nuclear measurements based on coupled neutron and gamma-ray transport.

The gamma flux-difference (GFD) method quantifies gamma-ray flux perturbations using exponential point kernels and Rytov approximations. Gamma-ray point kernels are corrected for flux buildup and flux perturbations caused by radial heterogeneities, i.e., standoff. Correction coefficients are calculated by flux-fitting one-dimensional (1D) radial sensitivity functions yielded by MCNP (Monte Carlo N-Particle code) to the 1D exponential gamma-ray kernel; they depend on standoff and mud density but are negligibly affected by formation properties.

The GFD method is benchmarked against Monte Carlo calculations. Compared to first-order approximations, it improves simulated density accuracy

across regions of significant contrasting properties, up to 0.1 g/cm^3 with 3.18-cm (1.25-in) standoff and freshwater mud. Gamma flux-difference approximations provide average density accuracy of 0.03 g/cm^3 up to 4.45-cm (1.75-in) standoff, similar to that of second-order forward modeling algorithms.

5.1 INTRODUCTION

In spatially complex formations, dipping layers, thin laminations, standoff, washouts, and/or invasion can mask true layer-by-layer formation properties measured with borehole nuclear tools. Inversion-based interpretation workflows can mitigate these 3D geometrical and borehole environmental effects along arbitrary well trajectories. They are based on forward numerical algorithms that incorporate measurement physics as well as borehole, tool, and formation geometry to simulate borehole nuclear measurements rapidly and accurately.

The Boltzmann transport equation governs neutron and gamma-ray transport. While simple to derive using principles of particle conservation, this equation cannot be solved analytically without severe practical limitations. Numerical methods need to be implemented instead, such as Monte Carlo (MC) algorithms with MCNP (Monte Carlo N-Particle code, Goorley, 2014). While flexible and accurate, Monte Carlo methods are computationally expensive, therefore inadequate for routine petrophysical analysis or inversion-based interpretation.

Solutions to the Boltzmann equation can also be approximated using Taylor series expansions and flux sensitivity functions (FSFs). Flux sensitivity functions were introduced by Watson (1984). Coupled with perturbation theory (Lewins, 1965; Greenspan, 1976), these functions can be used to simulate borehole nuclear

measurements in formations with perturbed properties (Watson, 1984, 1992; Couët and Watson, 1993; Case et al., 1994). Mendoza et al. (2007) accurately simulated borehole neutron and density measurements over a wide range of borehole conditions by combining first-order perturbation theory with Taylor series expansions. They also developed a linear iterative refinement (LIR) algorithm to select the optimal FSF background at each measured depth through iterative linear interpolations between pre-calculated, base-case, MC-derived flux sensitivity functions (Mendoza et al., 2010a, 2010b). Fast-forward models based on sensitivity functions and perturbation theory can be coupled with inversion procedures to achieve rapid and reliable petrophysical interpretation of well logs (Sanchez-Ramirez et al., 2009; Heidari et al., 2012, 2013; Ijasan et al., 2013b, 2014; Ajayi et al., 2015b; Ortega et al., 2017).

Across regions of significant contrasting properties, the accuracy of the LIR method decreases because spatial sensitivity flux perturbations introduce higher-order, nonlinear effects (with respect to changes in formation properties). Throughout this dissertation, higher-order effects refer to effects that cannot be accounted for using the first-term of a Taylor series expansion. More advanced methods have thus been developed based on second-order approximations for Gamma-Gamma density measurements (Zhou et al., 2009) or diffusion flux-difference (DFD) approximations for neutron measurements (Ijasan et al., 2013a).

For neutron porosity measurements, the diffusion flux-difference method quantifies spatial sensitivity flux perturbations using one-group neutron diffusion models. In the case of density porosity measurements, Zhou et al. (2009) calculated first- and second-order FSFs by implementing grid-by-grid perturbations using MCNP perturbation features. Sensitivity functions generated using grid-by-

grid perturbations tend to be coarse and oscillatory (Zhou et al., 2009). More importantly, MCNP only allows for perturbations in density, material composition, and reaction cross section data. Consequently, this technique can solely be applied for fast modeling of Gamma-Gamma density measurements, for which density is the characteristic perturbation parameter. Grid-by-grid perturbations in terms of migration length (the characteristic perturbation parameter for neutron-based measurements) or other complex perturbation parameters used to describe measurements based on two-particle transport, cannot be performed with MCNP.

I introduce a new method for Gamma-Gamma fast density modeling referred to as gamma flux-difference (GFD). This method quantifies gamma-ray flux perturbations based on gamma-ray point kernel approximations. It accurately models large flux perturbations such as those arising at the borehole wall in the presence of standoff. Borehole environmental effects are thus simulated within 0.02 g/cm³ accuracy up to 4.45-cm (1.75-in) standoff. This method was designed to be combined with diffusion flux-difference approximations to quantify flux perturbations on the measurements based on coupled neutron and gamma-ray transport, such as Neutron-Gamma density, or gamma-ray spectroscopy.

5.2 METHOD

5.2.1 Gamma-Ray Point Kernel Approximation

Gamma-ray flux sensitivity functions are computed by combining gamma-ray flux and gamma-ray importance functions derived respectively from forward and adjoint Boltzmann transport equations (Mendoza et al., 2010a), solved with the MCNP forward-adjoint generator (Booth and Hendricks, 1984). The forward

time-independent Boltzmann transport equation for a non-multiplying medium (i.e., the fission cross section is zero) is given by

$$[\mathbf{\Omega} \cdot \nabla + \mu_{T_0}(\mathbf{r}, E)] \Psi(\mathbf{r}, E, \mathbf{\Omega}) = \int dE' \int d\mathbf{\Omega}' \mu_s(\mathbf{r}, E\mathbf{\Omega} \rightarrow E'\mathbf{\Omega}') \Psi(\mathbf{r}, E', \mathbf{\Omega}') + S(\mathbf{r}, E, \mathbf{\Omega}) \quad (5.1)$$

where $\mathbf{r}$ is spatial coordinate, E is energy, $\mathbf{\Omega}$ is direction, defined by $\mathbf{\Omega} = \mathbf{v}/||\mathbf{v}||$, with $\mathbf{v}$ equal to gamma-ray velocity. The flux per unit energy and unit solid angle at position $\mathbf{r}$ is $\Psi(\mathbf{r}, E, \mathbf{\Omega})$, $\mu_{T_0}(\mathbf{r}, E)$ is total linear attenuation coefficient or total macroscopic cross section, $\mu_s(\mathbf{r}, E\mathbf{\Omega} \rightarrow E'\mathbf{\Omega}')$ is scattering cross section for scattering from energy E' to dE around E and from direction $\mathbf{\Omega}'$ to solid angle $d\mathbf{\Omega}'$ around $\mathbf{\Omega}$, and $S(\mathbf{r}, E, \mathbf{\Omega})$ is gamma-ray source density per unit energy and unit solid angle.

Perturbations to the sensitivity function caused by cross section perturbations can be quantified using an exponential point kernel derived from the Boltzmann transport equation. Assuming that the collision term, $\int dE' \int d\mathbf{\Omega}' \mu_s(\mathbf{r}, E\mathbf{\Omega} \rightarrow E'\mathbf{\Omega}') \Psi(\mathbf{r}, E', \mathbf{\Omega}')$, is zero in equation 5.1, and that the gamma-ray source is an isotropic monoenergetic point source located at $\mathbf{r}_s$, the transport equation for the uncollided gamma-ray flux, ψ^o , is written as

$$[\mathbf{\Omega} \cdot \nabla + \mu_{T_0}(\mathbf{r}, E)] \psi^o(\mathbf{r}, E, \mathbf{\Omega}) = S_0 \quad (5.2)$$

where S_0 is the source strength in particles per second. For the case of a monoenergetic isotopic point source placed at position $\mathbf{r}_s$, in a homogeneous

medium with total linear attenuation coefficient μ_{To} the uncollided gamma-ray flux in spherical coordinates [$\mathbf{r} = \mathbf{r}(r, \theta, \varphi)$] is therefore given by

$$\psi^o(\mathbf{r}) = S_0 \cdot \frac{\exp(-\mu_{To} |\mathbf{r} - \mathbf{r}_s|)}{4\pi |\mathbf{r} - \mathbf{r}_s|^2} = S_0 \cdot G^o(\mathbf{r}, \mathbf{r}_s) , \quad (5.3)$$

where $\exp(-\mu_{To} |\mathbf{r} - \mathbf{r}_s|)$ represents material attenuation, $1/4\pi |\mathbf{r} - \mathbf{r}_s|^2$ represents flux attenuation with increasing distance, also called geometric attenuation, and G^o is the uncollided exponential point kernel (also called Green's function) in an infinite homogeneous medium.

The uncollided point kernel model assumes no contribution from scattered or secondary gamma-rays, with the collision term set to zero in equation 5.1. Yet, scattered or secondary radiations contribute to flux buildup within the formation. To account for buildup, an additional term referred to as buildup factor is introduced in the expression (Chilton et al., 1984, Shultis and Faw, 1996). Thereafter, total gamma-ray point kernel is approximated as

$$G(\mathbf{r}, \mathbf{r}_s) = \frac{B(\mu_{To} |\mathbf{r} - \mathbf{r}_s|) \cdot \exp(-\mu_{To} |\mathbf{r} - \mathbf{r}_s|)}{4\pi |\mathbf{r} - \mathbf{r}_s|^2} , \quad (5.4)$$

where the buildup factor, $B(\mu_{To} |\mathbf{r} - \mathbf{r}_s|)$, adjusts the results for uncollided gamma-ray kernels to include contributions from collided particles, such as Compton scattered gamma-rays.

Three-dimensional cylindrical coordinates [$\mathbf{r} = \mathbf{r}(r, z, \theta)$] are better suited to describe the borehole geometry than spherical coordinates. Therefore, point

kernels are implemented in 3D cylindrical geometry using a transformation from cylindrical to spherical coordinates.

5.2.2 Buildup Effects

The buildup factor is estimated using the single-term Taylor form (Chilton et al., 1984) or single-term relaxation approximation (Shultis and Faw, 1996), given by

$$B(\mu_{T0}\mathbf{r}) \approx A_1 \exp(-\alpha_1 \mu_{T0} |\mathbf{r}|), \quad (5.5)$$

where parameters A_1 and α_1 depend on (a) gamma-ray energy, (b) atomic number of the attenuating medium, and (c) range $\mu_{T0}\mathbf{r}$ over which the approximation is used. By combining equations 5.4 and 5.5 I derive a new expression for gamma-ray point kernel, given by

$$G(\mathbf{r}, \mathbf{r}_s) \approx \frac{A_1 \exp[-\mu_{T0}(1+\alpha_1)|\mathbf{r}-\mathbf{r}_s|]}{4\pi|\mathbf{r}-\mathbf{r}_s|^2}. \quad (5.6)$$

5.2.3 Heterogeneous Medium

In enlarged boreholes, the point kernel must account for the presence of the heterogeneous radial layer of borehole mud, which causes increased gamma-ray flux attenuation within the formation. For example, if $\mathbf{r}_{BH}$ represents the position of the borehole wall in spherical coordinates between the source position, $\mathbf{r}_s$, and the observation point, $\mathbf{r}$, in direction $\boldsymbol{\Omega}$ (along the path of the particles), with $|\mathbf{r}-\mathbf{r}_{BH}| > 0$, the total gamma-ray point kernel reads

$$G(\mathbf{r}, \mathbf{r}_s, \mathbf{r}_{BH}) = \frac{B_{het}(\mathbf{r}) \exp\left[-(\mu_{To-Mud} |\mathbf{r}_{BH} - \mathbf{r}_s| + \mu_{To-Formation} |\mathbf{r} - \mathbf{r}_{BH}|)\right]}{4\pi |\mathbf{r} - \mathbf{r}_s|^2}, \quad (5.7)$$

where μ_{To-Mud} and $\mu_{To-Formation}$ are the total linear attenuation coefficients of the borehole mud and the formation, respectively, and B_{het} is the buildup factor of the heterogeneous medium. The point kernel expression in equation 5.7 requires generating new kernels for each borehole configuration, which takes several CPU hours, thus defying the purpose of fast modeling approximations. However, Shultis and Faw (1996) state that a medium can be “*homogenized conceptually*” when all materials have similar mass attenuations coefficients μ_m , with $\mu_m = \mu/\rho$. Because commonly encountered lithologies and borehole muds share nearly identical mass attenuation coefficients in the energy range of interest for Gamma-Gamma density tools (between 0.14 and 0.662 MeV), the final form of the point kernel is given by

$$G(\mathbf{r}, \mathbf{r}_s) \approx \frac{A_1 \exp(-\mu' |\mathbf{r} - \mathbf{r}_s|)}{4\pi |\mathbf{r} - \mathbf{r}_s|^2}, \quad (5.8)$$

where μ' is an effective linear attenuation coefficient that accounts for both presence of spatial heterogeneities and flux buildup.

At energy levels between 0.14 and 0.662 MeV, Compton scattering is the dominant interaction. The total linear attenuation coefficient, μ_{To} , is therefore approximated using the Compton linear attenuation coefficient per atom, μ_{Co} , such that

$$\mu_{To} \approx \mu_{Co} = {}_e\sigma_{Co} N_{Av} \rho_b \frac{Z}{A} = {}_e\sigma_{Co} N_{Av} \frac{\rho_e}{2}, \quad (5.9)$$

where ρ_e is electron density, ρ_b is bulk density, N_{Av} is Avogadro's number, σ_{Co} is Compton scattering cross section per electron, A is atomic mass, and Z is atomic number. The product $\sigma_{Co} N_{Av} / 2$ is constant and independent of rock composition, whereby equation 5.8 is rewritten in terms of modified electron density, α , such that

$$G(\mathbf{r}, \mathbf{r}_s) \approx \frac{A_1 \exp(-\alpha |\mathbf{r} - \mathbf{r}_s|)}{4\pi |\mathbf{r} - \mathbf{r}_s|^2}. \quad (5.10)$$

Modified electron density is determined by flux-fitting 1D radial sensitivity functions to the exponential point kernel in equation 5.10 for freshwater and gas-filled limestone, sandstone, and dolomite formations, in boreholes ranging from 21.6-cm (8.5-in) to 30.5-cm (12-in) diameter, with mud densities ranging from 1 g/cm³ (8.34 lbm/gal) to 2.5163 g/cm³ (21 lbm/gal). **Figure 5.1** shows cross-plots of modified electron density, α , and electron density, ρ_e , at long-spaced (panel a) and short-spaced (panel b) detectors. The relationship between modified electron density, α , and electron density, ρ_e , is given by

$$\alpha = \eta_1 \cdot \rho_e + \eta_2. \quad (5.11)$$

Correction coefficients η_1 and η_2 vary with detector position, standoff, and borehole mud density, but are independent of formation rock composition (**Figure 5.1**). Modified electron density, α , is smaller than electron density because of flux buildup. It is also smaller at the long-spaced detector (LSn) compared to the short-spaced detector (SSn) to account for the increased probability of scattering

interactions (increased flux buildup) over longer distances. Modified electron density increases with increasing standoff because the heterogeneous layer of mud causes increased flux buildup inside the borehole, thus increasing gamma-ray flux attenuation within the formation.

Corrections coefficients η_1 and η_2 were calculated for boreholes ranging from 21.6-cm (8.5-in) to 30.5-cm (12-in) diameter, with mud densities ranging from 1 to 2.5163 g/cm³ (**Figure 5.1**). Based on these results, **Figure 5.2** shows 2D interpolation maps of correction coefficients η_1 and η_2 with respect to standoff, and to the electron density of the borehole mud, whereby the modified electron density, α , can be calculated for arbitrary combinations of mud density and standoff (up to 4.45 cm or 1.75 in).

5.2.4 Rytov Approximation and Gamma-Ray Flux-Differences (GFD) Distributed Functions

When implementing a first-order Rytov approximation (Habashy et al., 1993), the perturbed sensitivity function FSF_{GFD} for an earth model associated with the modified cross section parameter, $\alpha(\mathbf{r})$, is given by (Ijase et al., 2013a)

$$\log_e FSF_{GFD}(\mathbf{r}_R, \mathbf{r}) \approx \frac{J_b(\mathbf{r})}{\Gamma_b(\mathbf{r})} [\alpha(\mathbf{r}) - \alpha_b] + \log_e FSF_b(\mathbf{r}_R, \mathbf{r}) , \quad (5.12)$$

where $FSF_b(\mathbf{r}_R, \mathbf{r})$ is the MC-derived sensitivity function for the homogeneous background (reference) medium, b , for detector R located at $\mathbf{r}_R$. The distributed flux, Γ_b , is an analytical approximation of the base-case sensitivity function, FSF_b , derived from the point kernel equation, and J_b is the derivative of the point kernel distributed flux, Γ_b , with respect to the background modified parameter, α_b .

According to the point kernel approximation, the flux, Γ , generated by a distributed source can be decomposed into contributions from individual point sources (Glasstone and Sesonske, 1994), i.e.,

$$\Gamma(\mathbf{r}) = \int d\mathbf{r}_s S(\mathbf{r}_s) G(|\mathbf{r} - \mathbf{r}_s|), \quad (5.13)$$

where $S(\mathbf{r}_s)$ is the strength of a radiation source located at $\mathbf{r}_s$ and G is the point kernel that represents the detector response at space point $\mathbf{r}$. The base-case sensitivity function, FSF_b , is regarded as a distributed source whose behavior is described by equation 5.13, such that

$$Gfd_b(\mathbf{r}) = \frac{J_b(\mathbf{r})}{\Gamma_b(\mathbf{r})} = \frac{\int d\mathbf{r}_s FSF_b(\mathbf{r}_R, \mathbf{r}_s) \frac{dG_b}{d\alpha_b}(c)}{\int d\mathbf{r}_s FSF_b(\mathbf{r}_R, \mathbf{r}_s) G_b(\mathbf{r}, \mathbf{r}_s)}, \quad (5.14)$$

where Gfd_b is the base-case gamma flux-difference (GFD) distributed function.

The point kernel G_b is calculated from equation 5.10 with the background modified electron density, α_b , such that

$$G_b(\mathbf{r}, \mathbf{r}_s) \approx \frac{A_1 \exp(-\alpha_b |\mathbf{r} - \mathbf{r}_s|)}{4\pi |\mathbf{r} - \mathbf{r}_s|^2}, \quad (5.15)$$

and its derivative is given by

$$\frac{dG_b}{d\alpha_b}(\mathbf{r}, \mathbf{r}_s) \approx \frac{-A_1 \operatorname{sgn}(|\mathbf{r} - \mathbf{r}_s|) \exp(-\alpha_b |\mathbf{r} - \mathbf{r}_s|)}{4\pi |\mathbf{r} - \mathbf{r}_s|}, \quad (5.16)$$

The unknown parameter A_1 cancels out in equation 5.14 because it is present in both the denominator and the numerator, i.e., the gamma-ray point kernel and its derivative, respectively.

Figure 5.3 displays background spatial FSF and GFD functions at long- (top panels), and short-spaced (bottom panels) detectors in a freshwater-filled 5 porosity units (p.u.) limestone formation. Panels (b) and (h) show the distributed point kernel gamma-ray flux, Γ_b , derived from equation 5.13 where the background MC-derived sensitivity function, FSF_b , (panels a and g) is the distributed gamma-ray source, $S(\mathbf{r}_s)$. To qualitatively assess the exponential point kernel model, I compare normalized 1D projections of Γ_b (dashed red line) and FSF_b (solid red line), in vertical (panels e and k) and radial (panels f and l) directions. The agreement between Γ_b and FSF_b is superior at the long-spaced gamma-ray detector (panel k) because the geometric attenuation becomes more accurate at greater distances from the source. The derivative of the distributed point kernel gamma-ray flux, J_b , (panels c and j) is negative, which validates the decrease of gamma-ray flux (attenuation increases) as the modified electron density, α , increases. Gamma-ray flux-difference distributed functions, $Gfd_b = J_b / \Gamma_b$, (panels d and j), and sensitivity functions, FSF_b , are saved as base cases to compute perturbed sensitivity functions, FSF_{GFD} (equation 5.12).

5.2.5 Boundary Conditions

In equation 5.12, flux continuity is enforced by the condition

$$\left. \frac{J_b}{\Gamma_b} \Delta\alpha(\mathbf{r}) \right|_{\mathbf{r}=\mathbf{r}_{bd}-\epsilon} = \left. \frac{J_b}{\Gamma_b} \Delta\alpha(\mathbf{r}) \right|_{\mathbf{r}=\mathbf{r}_{bd}+\epsilon} \quad \forall \quad \mathbf{r} > \mathbf{r}_s \quad (5.17)$$

at locations, $\mathbf{r}_{bd}$, where the perturbation $\Delta\alpha(\mathbf{r}) = \alpha(\mathbf{r}) - \alpha_b$ exhibits a discontinuity caused by the borehole wall, formation boundaries, or/and invasion front, i.e., $\Delta\alpha(\mathbf{r}_{bd} + \epsilon) \neq \Delta\alpha(\mathbf{r}_{bd} - \epsilon)$ for $\epsilon \rightarrow 0$.

5.2.6 Detector Response Perturbation

Upon calculation of the perturbed sensitivity function, FSF_{GFD} , (equation 5.12), and after enforcing flux continuity (equation 5.17), the perturbed detector response N is determined using the Taylor series expansion (Ijasaan et al., 2013a)

$$N \approx N_b + N_b \int d\mathbf{r} \quad FSF_b(\mathbf{r}) \frac{\Delta\alpha(\mathbf{r})}{\alpha_b} + N_b \int d\mathbf{r} \quad \Delta FSF(\mathbf{r}) \frac{\alpha(\mathbf{r})}{\alpha_b}, \quad (5.18)$$

where $\Delta FSF = FSF_{GFD} - FSF_b$ represents the flux perturbation due to $\Delta\alpha$ calculated with the gamma-ray point kernel approximation, and N_b is base-case detector response. The detector response, N , is proportional to the number of particles entering the detector per unit time (particle count rate). **Figure 5.4** describes the full workflow used to simulate long-, ρ_{LS} , and short-spaced, ρ_{SS} , density via gamma flux-difference approximations. On one hand, the dashed green rounded rectangle in **Figure 5.4** describes the 1D flux-fitting process used to compute 2D interpolation maps for the correction coefficients η_1 and η_2 , depending on standoff and mud density. On the other hand, the dashed purple rounded rectangle details the implementation of gamma-ray point kernel approximations to compute base-case GFD distributed functions, Gfd_b . Base-case GFD distributed functions, and base-case FSFs are calculated for the homogeneous formations listed in **Table 5.1** and stored in a library for subsequent use. The library, identified by a dashed

blue rounded rectangle, also includes pre-computed 2D maps for corrections coefficients η_1 and η_2 . At each measured depth, the fast-forward model (dashed red rounded rectangle) simulates perturbed detector counts with respect to a background case, selected from existing library base-cases (**Table 5.1**) such that $\Delta\alpha$ is minimized in a least-squares sense.

5.3 BENCHMARK RESULTS

The gamma flux-difference algorithm is implemented and benchmarked for a generic dual-detector LWD density tool with a cesium-137 gamma-ray source, and a 21.6-cm (8.5-in) drill collar. Short- and long-spaced gamma detectors are located 21.6 cm (8.5 in) and 41.9 cm (16.5 in) from the source, respectively (Ijasan et al., 2011).

5.3.1 Homogeneous Formations

Perturbed gamma flux-difference sensitivity functions, FSF_{GFD} , are generated for homogeneous formation perturbations with the first-order Rytov approximation (equation 5.12). The background sensitivity function, FSF_b , is constructed for a 0 p.u. limestone formation using MCNP. **Figure 5.5** compares qualitatively FSF_{GFD} and FSF_{MC} (perturbed Monte Carlo FSFs) across freshwater and gas-filled limestone formations. In the presence of homogeneous perturbations resulting from variations in porosity and fluid composition, the qualitative comparisons indicate that the gamma flux-difference method is a good approximation to Monte Carlo calculations for homogeneous perturbations of up to 0.2 g/cm³.

5.3.2 Effect of Standoff

In the presence of standoff, Zhou et al. (2009) showed that second-order approximations provide a density accuracy of 0.02 g/cm³ and 0.03 g/cm³ at long- and short-spaced detectors, respectively. Density accuracy is improved by as much as 70% when compared to first-order approximations (Zhou et al., 2009). The gamma flux-difference method yields similar results, for both centered and eccentric tool configurations; its efficiency is compared to that of the linear iterative refinement (LIR) method (Mendoza et al., 2007) which implements first-order approximations, coupled with an iterative process to minimize density perturbations when selecting background sensitivity functions.

5.3.2.1 *Centered Tool Configuration*

I studied the effect of standoff in enlarged boreholes for centered tool configurations. **Figure 5.6** compares density calculated with LIR and GFD sensitivity functions to density derived from MCNP counts in freshwater and gas-filled limestone formations for increasing values of standoff. The gamma flux-difference method yields errors of 0.02 g/cm³ or less at long- and short-spaced gamma-ray detectors, up to 4.45-cm (1.75-in) standoff. Conversely, the linear iterative refinement algorithm overestimates density up to 0.1 g/cm³ when formation and borehole mud involve large density contrasts, such as low-porosity (high-density) formations coupled with freshwater mud. **Figures 5.7 and 5.8** qualitatively compare MC-derived sensitivity functions, and perturbed GFD and LIR sensitivity functions in a 26.7-cm (10.5-in) borehole (1-in standoff) for freshwater (1 g/cm³) and 66 wt% barite muds (2.0440 g/cm³), respectively. The 1D radial projection of MC-derived sensitivity function (panels c and g) shows that gamma-ray flux exhibits significant attenuation upon exiting the borehole,

specifically when the contrast between mud and formation electron density increases. Indeed, gamma-ray flux attenuation is stronger in materials with high electron density (equation 5.10). Buildup effects must also be considered: materials with low atomic number, Z , (usually associated with low density) tend to increase the relative abundance of low-energy gamma rays through Compton scattering, whereas higher Z materials exhibit stronger photoelectric effects. Consequently, low-energy gamma-ray flux builds up inside the borehole. Upon entering the formation (higher Z material), low-energy gamma rays are more likely to undergo photoelectric absorption, and gamma-ray flux decreases abruptly. Projections in the radial direction (1D) show that the LIR method does not capture such gamma-ray attenuation effects, thereby overestimating the simulated density. Conversely, sensitivity functions calculated using gamma flux-difference approximations accurately quantify flux perturbations resulting from standoff, in both radial and vertical directions. Density accuracy is therefore improved by as much as 80% when compared to the LIR method.

5.3.2.2 Eccentered Tool Configuration

Gamma flux-difference approximations provide similar density accuracies with eccentered tool configurations. In 25.4-cm (10-in, **Figure 5.9**) and 30.5 (12-in, **Figure 5.10**) boreholes, the gamma flux-difference method delivers accuracies of 0.03 g/cm^3 for freshwater and gas-filled limestone formations of 30 p.u. or less, independently of tool orientation. **Figure 5.11** compares the sensitivity functions in three dimensions (panels a, f, and b, g), and in the vertical and radial directions (panels c, h, and d, i); GFD approximations capture the decrease in gamma-ray flux at the borehole wall, whereas LIR sensitivity functions tend to overestimate the

importance of the formation. It is also worth noting that the decrease in gamma-ray flux is emphasized when standoff increases because buildup of low-energy gamma rays increases in low-Z materials.

5.3.3 Effect of Invasion

Invasion fronts also act as boundaries between materials of contrasting properties. However, flux perturbations occurring at invasion fronts are not as significant because the contrast in material properties merely reflects the corresponding change in pore fluid composition. I studied a piston-like invasion of freshwater mud in a 30 p.u. gas-filled (methane with a bulk density of 0.0178 g/cm^3) limestone formation (**Figure 5.12**). Densities of flushed and virgin zones are 2.197 g/cm^3 and 1.9023 g/cm^3 , respectively. Simulated densities computed using LIR (solid green line), GFD (dashed blue line), and MCNP (red markers) algorithms are plotted against invasion depth at long- (panel a), and short-spaced (panel b) detectors. Panel (c) shows compensated density, ρ_{CO} , and panel (d), misfit vs. invasion depth. The advantage of the GFD method over the LIR algorithm is mainly observed for shallow invasion. Between 2.5 and 5.1 cm (1 and 2 in), gamma flux-difference approximations improve density accuracy by 0.02 g/cm^3 when compared to the LIR method.

5.3.4 Modeling the Effect of Invasion in a High-Angle Well

In high-angle wells, gamma rays sense dipping bed boundaries as radial perturbations, thus causing flux perturbations in the radial direction. Mud filtrate invasion is affected by gravity and tends to follow a non-symmetrical “teardrop” invasion profile. I study the combined effects of invasion and deviated beds with one synthetic example featuring an 85° deviated well with no standoff. Formation

layers have a true stratigraphic thickness (TST) of 39.6 cm (1.3 ft) and are invaded with oil-base mud (OBM, $C_{14}H_{30}$, 0.8 g/cm^3). Their composition and properties are listed in **Table 5.2**. The “teardrop” invasion profile is approximated by 3D eccentric cylinders. This synthetic case is taken from Ijase et al. (2013a) who compared LIR and DFD algorithms for neutron measurements. Layer I is a 5 p.u. shale formation with shallow invasion, and layers II and III are 5 and 30 p.u. gas-bearing sandstones, respectively, with deeper invasion in Layer II. Layers IV and V are 30, and 5 p.u. water-filled sandstones, with deeper invasion in layer V.

In **Figure 5.13**, I compare LIR and GFD approximations, but also illustrate the combined benefits of DFD and GFD algorithms. The earth model is described in panel (a) in terms of bulk density. Panel (b) shows a borehole image of neutron porosity simulated using diffusion flux-difference approximations. Borehole images of simulated density using LIR, GFD, and MCNP algorithms are shown in panels (c), (d), and (e), respectively. Measurement transition at bed boundaries is accurately simulated by the GFD method while the LIR algorithm tends to sharpen the transition. Residuals of simulated densities with respect to MC-derived densities (panels h and i) show that the GFD algorithm provides minimum accuracy of 0.03 g/cm^3 in all azimuthal sectors. The average error per depth is improved up to 0.045 g/cm^3 (panel j) when compared to the LIR algorithm. **Figure 5.14** qualitatively compares LIR, GFD, and MC-derived sensitivity functions. In panels (c) and (g), the GFD-perturbed sensitivity function captures the small increase in sensitivity caused by the combined influences of invasion and dipping bed boundary at 12.2 m (40.16 ft, measured depth).

It is also worth noting that nonlinear effects are not as common in density measurements compared to neutron measurements. For density measurements,

flux perturbations subject to higher-order effects more readily occur in the presence of standoff than invasion or dipping layers. Accordingly, in this synthetic example, the combined use of GFD and DFD algorithms (**Figure 5.13f**) improves porosity estimates by as much as 10 p.u. for DFD and 2.5 p.u. for GFD.

5.4 DISCUSSION

The gamma flux-difference method quantifies flux perturbations resulting from sharp contrasts in electron density. It was implemented and benchmarked with an LWD density tool, but its principles can be readily applied to wireline measurements. When modeling borehole environmental effects, density accuracy is 0.02 g/cm³ up to 4.45-cm (1.75-in) standoff, significantly improved compared to that of the linear iterative refinement algorithm (0.1 g/cm³). In deviated wells, and in the presence of invasion, the gamma flux-difference method for density measurements can be used in combination with diffusion flux-difference approximations for neutron measurements to deliver more accurate petrophysical interpretations. The GFD algorithm is at least 1,000 times faster than MCNP with one sample point simulated in 0.15 seconds. It is also more versatile than the LIR method which requires an extensive database to simulate a limited number of cases. From base cases in **Figure 5.5**, listed in **Table 5.1**, the GFD method can generate flux sensitivity functions for any borehole size, borehole mud, tool eccentricity, and orientation, whereas the LIR method requires a library with more than 100 precalculated MC-derived FSFs.

The GFD method accounts for buildup and heterogeneity effects in the presence of standoff with correction coefficients η_1 and η_2 , which are calculated by

flux-fitting 1D radial sensitivity functions to the exponential point kernel for several values of standoff and mud density. However, when calculating gamma flux-difference distributed functions, Gfd_b , the GFD algorithm assumes that buildup and heterogeneity effects resulting from discontinuities within the formation, such as invasion fronts or bed boundaries, are negligible. This assumption allows for rapid implementation of the gamma flux-difference method (perturbed FSF are calculated in 0.015 seconds), because GFD functions are pre-computed independently of formation geometry and stored for subsequent use. **Figure 5.14** shows that flux perturbations are accurately simulated without considering buildup or heterogeneity effects resulting from the invasion front or the dipping bed boundary.

The gamma flux-difference method provides density accuracy similar to that achieved by Zhou et al. (2009) whose fast-forward model is based on second-order approximations. Zhou et al. constructed first- and second-order sensitivity functions using a perturbation feature available in MCNP. Because this process is extremely computationally expensive, the sensitivity maps tend to be coarse and to exhibit numerical oscillations. MCNP also limits perturbations to material composition, cross sections, and bulk density. Consequently, MCNP cannot be used to derive second-order sensitivity maps for measurements based on two-particle transport.

Conversely, the GFD method was designed to be combined with DFD to quantify flux perturbations on measurements based on coupled neutron and gamma-ray transport. Another similar solution is to develop a flux-difference algorithm based on coupled-field theory.

5.5 CONCLUSIONS

I developed a new method to simulate borehole Gamma-Gamma density measurements across challenging logging environments, including enlarged boreholes. Similarly to first-order numerical simulations (such as the linear iterative refinement method), this algorithm is based on Monte Carlo pre-computed base-case sensitivity functions. Additionally, it introduces a higher-order perturbation term to account for spatial sensitivity flux perturbations arising at boundaries between layers with sharp contrasts in electron density. Perturbed sensitivity functions are calculated using an exponential gamma-ray point kernel model coupled with a Rytov approximation. Empirical correction coefficients account for flux buildup and non-negligible flux perturbations arising in the presence of standoff; they vary with mud density and standoff but are independent of rock composition.

In enlarged boreholes and with low-density mud, gamma-ray sensitivity functions exhibit significant attenuation at the borehole wall. Qualitative comparisons show that gamma flux-difference approximations accurately reproduce this behavior, while the LIR algorithm systematically overestimates the magnitude of the sensitivity flux within the formation. Consequently, the LIR method overestimates density up to 0.1 g/cm^3 , while GFD accuracy is within 0.03 g/cm^3 . Flux perturbations of smaller magnitude also occur with invasion or in the presence of dipping layers. In deviated wells with invaded beds, the GFD algorithm improves average density accuracy up to 0.045 g/cm^3 ($\sim 2.5 \text{ p.u.}$) when compared to the LIR method and delivers borehole images that reproduce shoulder-bed effects more accurately.

Simulations obtained with the LIR method have low accuracy when they yield sensitivity functions that significantly differ from library base-case FSFs. For example, at the short-spaced detector, LIR approximations yield 0.1 g/cm³ error for 3.18-cm (1.25-in) standoff with freshwater mud. Consequently, FSF libraries for LIR fast-forward simulations typically require more than 100 cases. The new GFD algorithm circumvents the cumbersome process of pre-computing sensitivity functions for diverse tool/borehole configurations: perturbed sensitivity functions were calculated from eight base-case FSFs, in milliseconds of CPU time, for an infinite number of borehole sizes, borehole muds, tool eccentricities, and orientations.

In uncompensated measurements, borehole environmental corrections based on empirical relationships might depend on formation properties, and require a-priori knowledge of standoff, eccentricity, and mud type. Inversion-based borehole environmental corrections could be implemented instead if flux perturbations resulting from standoff were accurately quantified. The gamma flux-difference method is the first step toward such improvements: compared to fast-forward models based on second-order approximations, it can be combined with diffusion flux-difference approximations to simulate borehole environmental effects on measurements based on coupled neutron and gamma-ray transport, such as Neutron-Gamma density, and gamma-ray spectroscopy.

Base-case description	Volumetric concentrations [v/v]	Bulk density, ρ_b [g/cm ³]	Electron density, ρ_e [g/cm ³]
FW LI - 0 p.u.	0.00 H ₂ O 1.00 CaCO ₃	2.7100	2.7076
FW LI - 5 p.u.	0.05 H ₂ O 0.95 CaCO ₃	2.6245	2.6278
FW LI - 10 p.u.	0.10 H ₂ O 0.90 CaCO ₃	2.5390	2.5479
FW LI - 20 p.u.	0.20 H ₂ O 0.80 CaCO ₃	2.3680	2.3881
FW LI - 30 p.u.	0.30 H ₂ O 0.70 CaCO ₃	2.1970	2.2284
CH ₄ [0.0178 g/cm ³] LI - 20 p.u.	0.20 CH ₄ 0.70 CaCO ₃	2.1716	2.1705
FW LI - 40 p.u.	0.40 H ₂ O 0.60 CaCO ₃	2.0260	2.0687
CH ₄ [0.0178 g/cm ³] LI - 30 p.u.	0.30 CH ₄ 0.70 CaCO ₃	1.9023	1.9020

Table 5.1. Description of homogeneous formation base-cases used to compute MC-derived sensitivity function base-cases, FSF_b , and gamma flux-difference distributed functions, Gfd_b , base cases.

Layer	Approximate "teardrop" invasion profile geometry		Volumetric concentrations [v/v]		Bulk density, ρ_b [g/cm ³]	
	Invasion radius [cm]	Cylinder eccentered distance [cm]	Invaded zone	Virgin zone	Invaded zone	Virgin zone
I	16	4.35	0.05 C ₁₄ H ₃₀ 0.40 SiO ₂ 0.50 Al ₂ Si ₂ O ₅ (OH) ₄ 0.05 FeS ₂	0.05 H ₂ O 0.40 SiO ₂ 0.50 Al ₂ Si ₂ O ₅ (OH) ₄ 0.05 FeS ₂	2.5850	2.6655
II	27	4.35	0.05 C ₁₄ H ₃₀ (0.0178g/cm ³) 0.95 SiO ₂	0.05 CH ₄ (0.0178g/cm ³) 0.95 SiO ₂	2.5575	2.5184
III	20	4.35	0.30 C ₁₄ H ₃₀ (0.0178g/cm ³) 0.70 SiO ₂	0.30 CH ₄ (0.0178g/cm ³) 0.70 SiO ₂	2.0950	1.8603
IV	20	4.35	0.30 C ₁₄ H ₃₀ 0.70 SiO ₂	0.30 H ₂ O 0.70 SiO ₂	2.0950	2.1550
V	27	4.35	0.05 C ₁₄ H ₃₀ 0.95 SiO ₂	0.05 H ₂ O 0.95 SiO ₂	2.5575	2.5675

Table 5.2: Layer properties of the synthetic earth model for the approximate “teardrop” invasion profile.

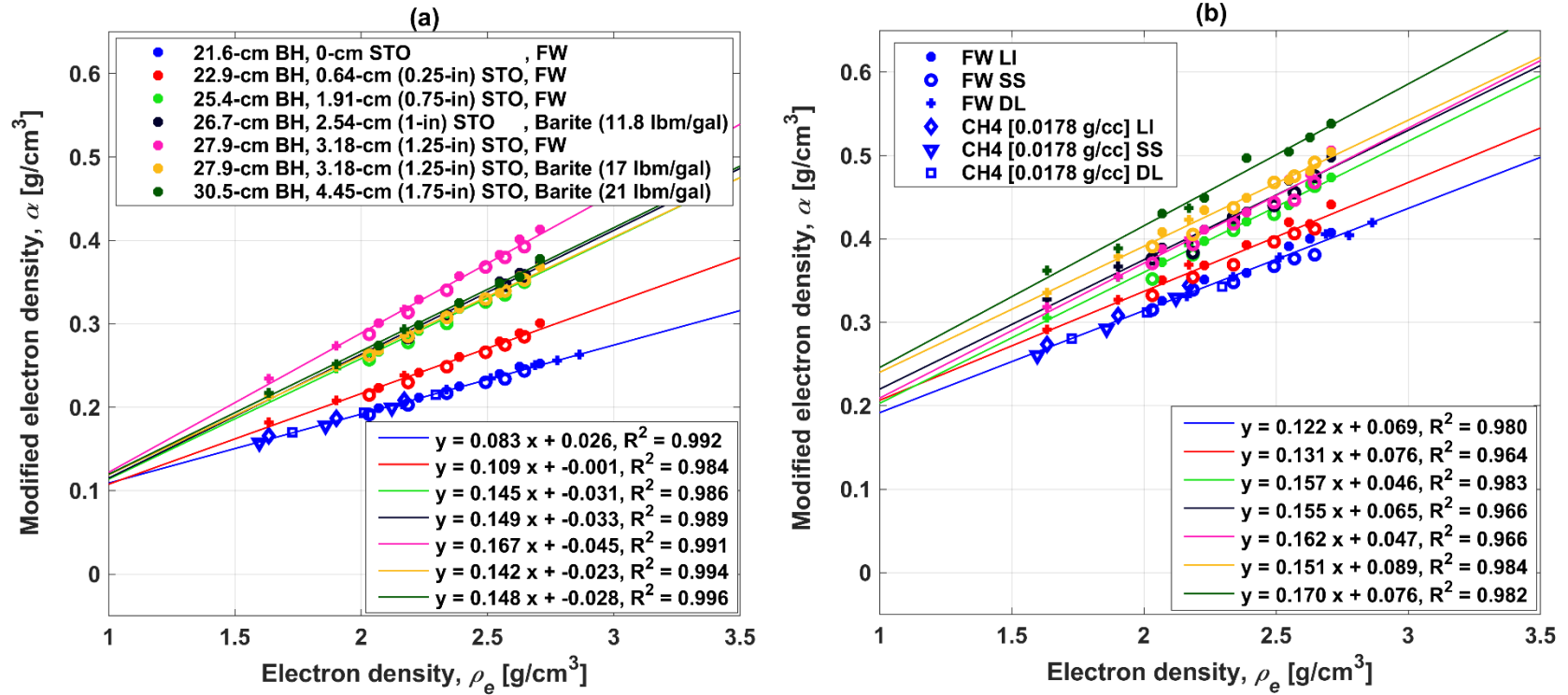


Figure 5.1. Cross-plot of modified electron density, α , and electron density, ρ_e , at (a) long- and (b) short-spaced detectors for freshwater and gas-filled limestone, sandstone, and dolomite formations, for boreholes with diameters ranging from 21.6 to 30.5 cm (8.5 to 12 in), and with mud density ranging from 1 g/cm^3 (8.3 lbm/gal) to 2.5163 g/cm^3 (21 lbm/gal).

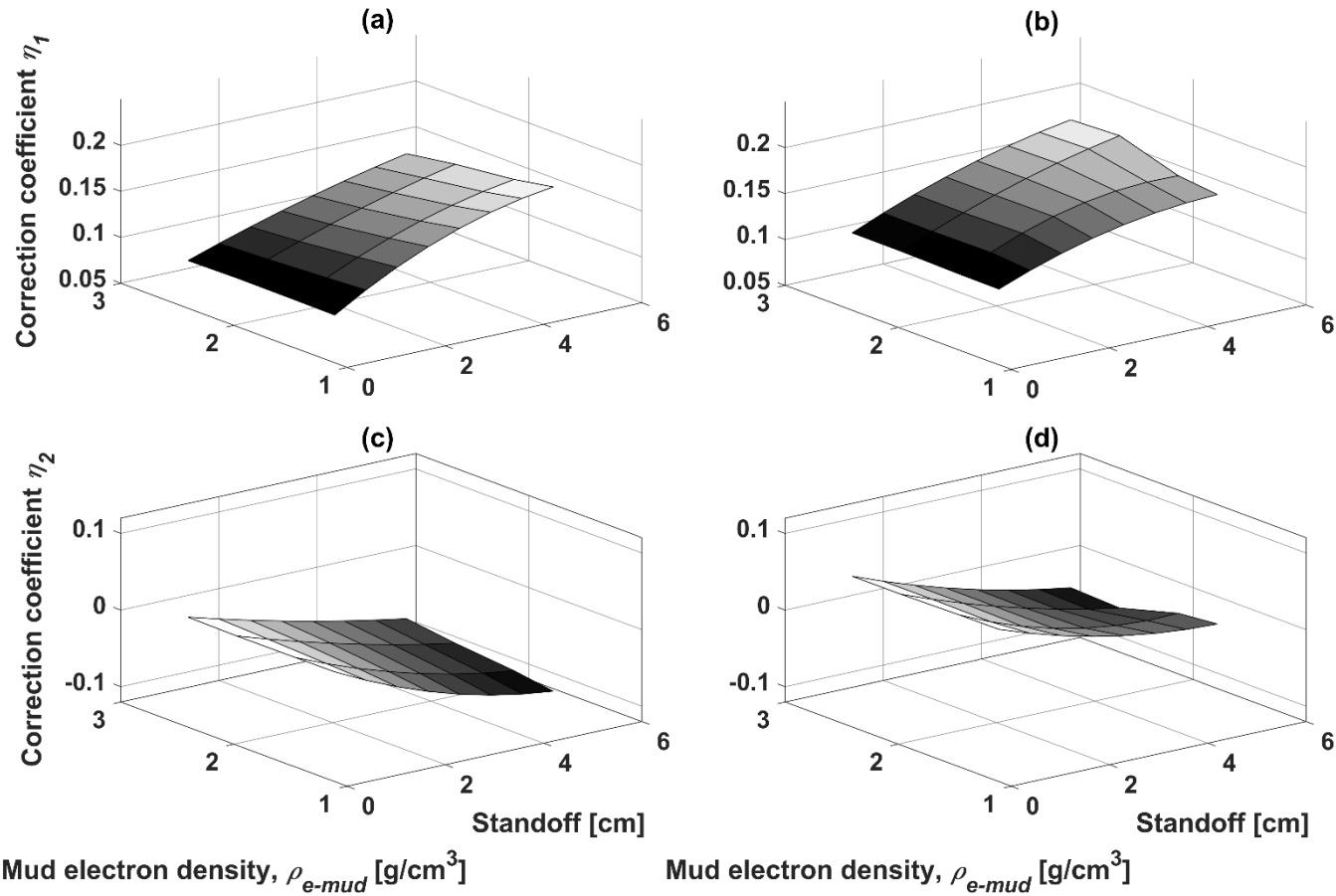


Figure 5.2. Correction coefficients η_1 and η_2 with respect to standoff, and to electron density of borehole mud, at long- (left panels) and short-spaced (right panels) detectors. Correction coefficient η_1 at (a) long- and (b) short-spaced detectors, and correction coefficient η_2 at (c) long- and (d) short-spaced detectors.

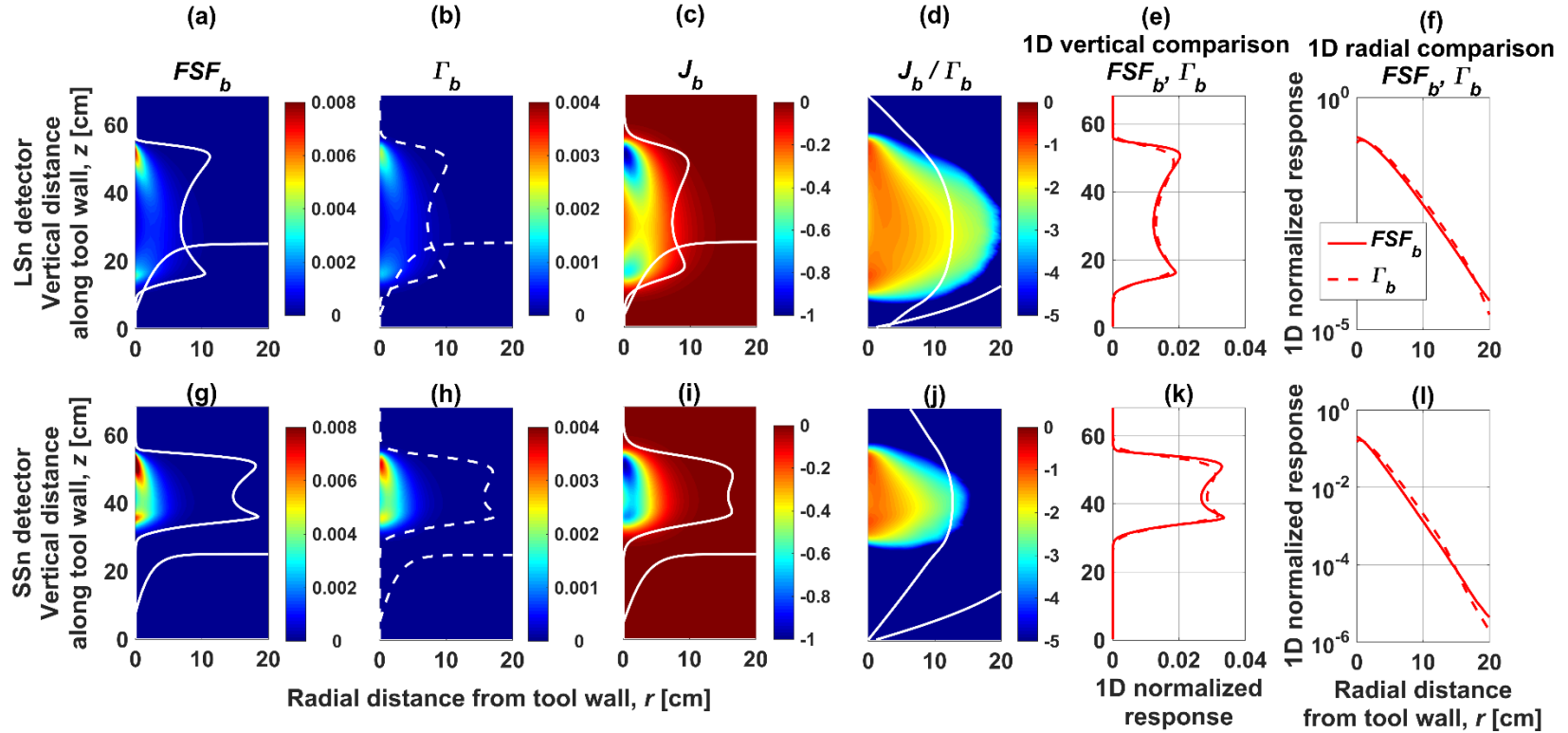


Figure 5.3. Description of background spatial FSF and GFD functions at long- (top panels), and short-spaced (bottom panels) detectors in a freshwater-filled 5 p.u. limestone formation. (a)(g) MC-derived background sensitivity function, FSF_b ; (b)(h) distributed point kernel gamma-ray flux, Γ_b ; (c)(i) derivative of the distributed point kernel gamma-ray flux, J_b ; and (d)(j) gamma-ray flux-difference distributed function, $Gfd_b = J_b / \Gamma_b$. Colors describe the relative 2D spatial sensitivity, with white lines identifying 1D vertical projections, and radial J-functions. Qualitative 1D comparison between FSF_b (solid red lines), and Γ_b (dashed red lines) at long- (top panels), and short-spaced (bottom panels) detectors in a freshwater-filled 5 p.u. limestone formation, with (e)(k) vertical projections integrated in the azimuthal and radial directions; and (f)(l) radial projections integrated in the azimuthal and vertical directions.

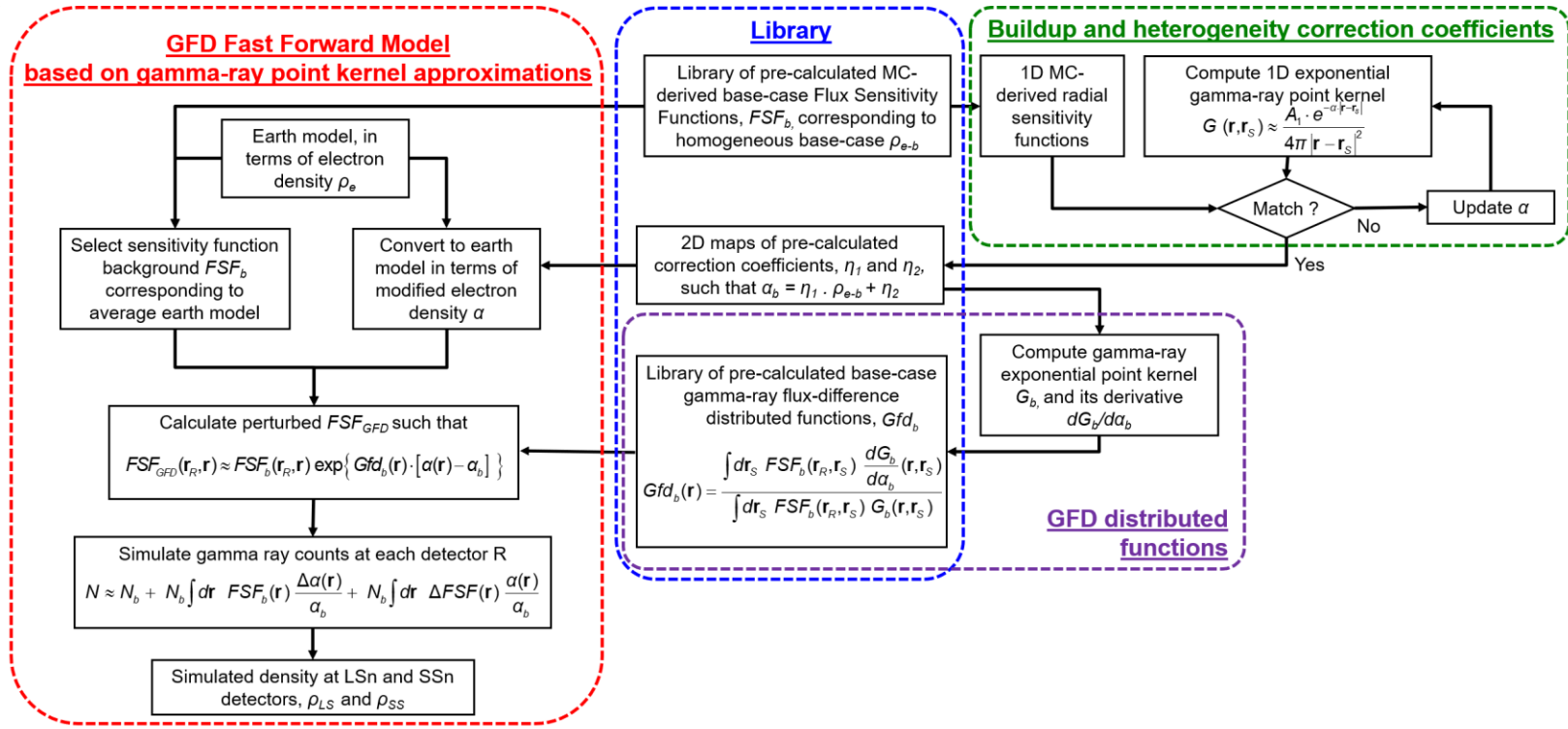


Figure 5.4. Flow diagram describing the implementation of the GFD fast-forward model. The dashed green rounded rectangle identifies the 1D flux-fitting process to calculate modified electron density, α , for different rock compositions, standoff values, and mud densities, and to generate 2D interpolation maps for correction coefficients η_1 and η_2 . The dashed purple rounded rectangle identifies the process of calculating base-case gamma flux-difference (GFD) distributed functions based on gamma-ray point kernel approximations. Pre-computed corrections coefficients η_1 and η_2 , base-case GFD distributed functions, and base-case FSFs are stored in a library (identified by a dashed blue rounded rectangle), with the base-case formations listed in **Table 5.1**. The fast-forward algorithm (identified by a dashed red rounded rectangle) simulates perturbed detector counts at each depth by selecting optimal background FSF and GFD functions from the library.

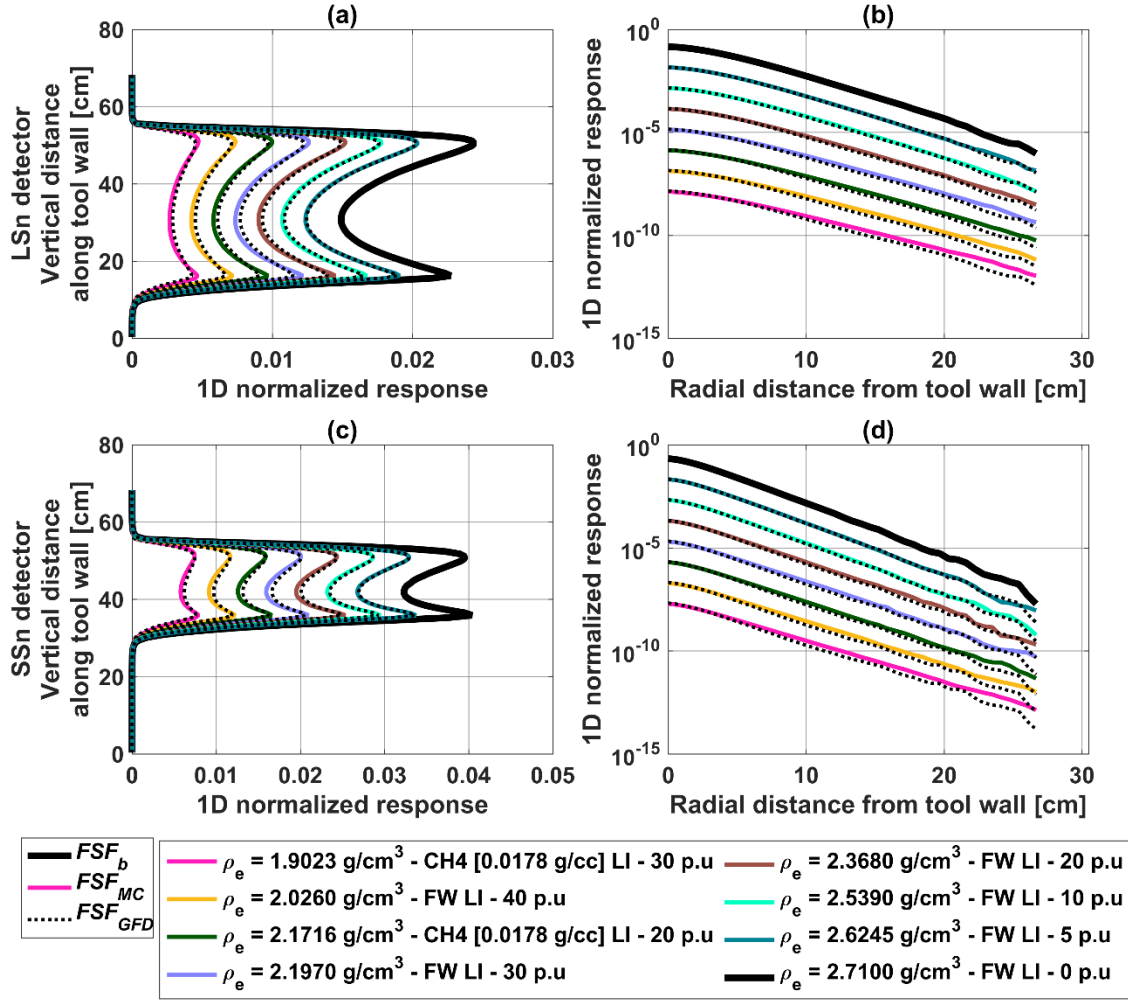


Figure 5.5. Qualitative comparison of MC-derived and perturbed gamma flux-difference sensitivity functions in freshwater and gas-filled limestone homogeneous formations. Left- and right-hand panels show 1D sensitivity functions projected in the vertical and radial directions, respectively. Top and bottom panels show sensitivity functions at long- and short-spaced detectors, respectively. MC-derived perturbed sensitivity functions FSF_{MC} are identified by solid lines with MC-derived background sensitivity function FSF_b in black. Black dashed lines display perturbed sensitivity functions, FSF_{GFD} , calculated from background FSF_b using gamma-ray point kernel approximations. (a) Sensitivity functions integrated in the azimuthal and radial direction at the long-spaced detector. (b) Sensitivity functions integrated in the azimuthal and vertical direction at the long-spaced detector. (c) Similar to (a) at the short-spaced detector. (d) Similar to (b) at the short-spaced detector.

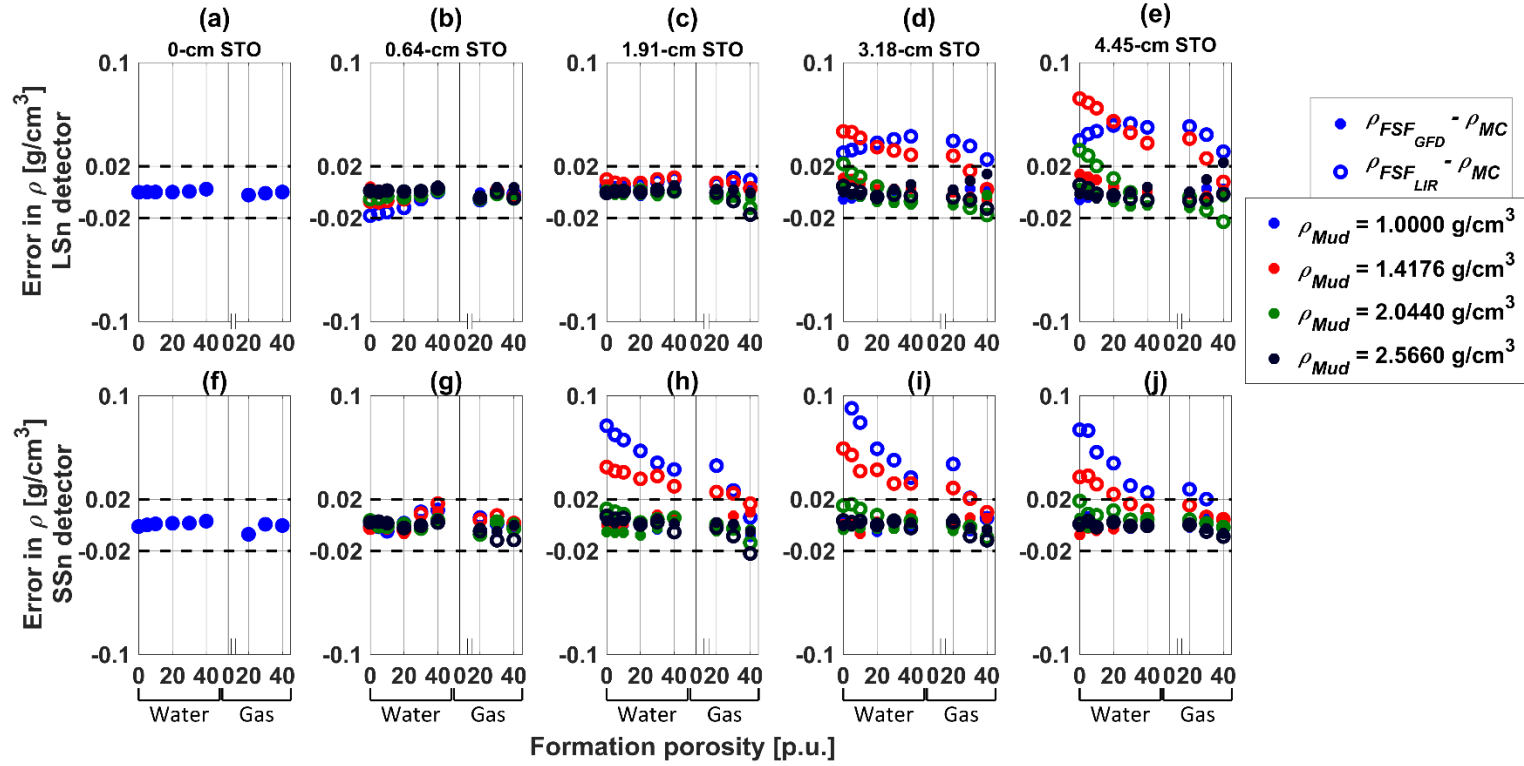


Figure 5.6. Density accuracy at long- (top panels) and short-spaced (bottom panels) detectors in freshwater and gas-filled limestone formations for (a)(f) 0-cm, (b)(g) 0.64-cm (0.25-in), (c)(h) 1.91-cm (0.75-in), (d)(i) 3.18-cm (1.25-in), and (e) 4.45-cm (1.75-in) of standoff (centered tool configuration), with borehole mud densities between 1 and 2.5660 g/cm³. Density errors are calculated with respect to densities estimated from MCNP gamma-ray counts, ρ_{MC} . Point and circle markers identify errors for densities calculated using the GFD method, $\rho_{FSF_{GFD}}$, and LIR method, $\rho_{FSF_{LIR}}$, respectively.

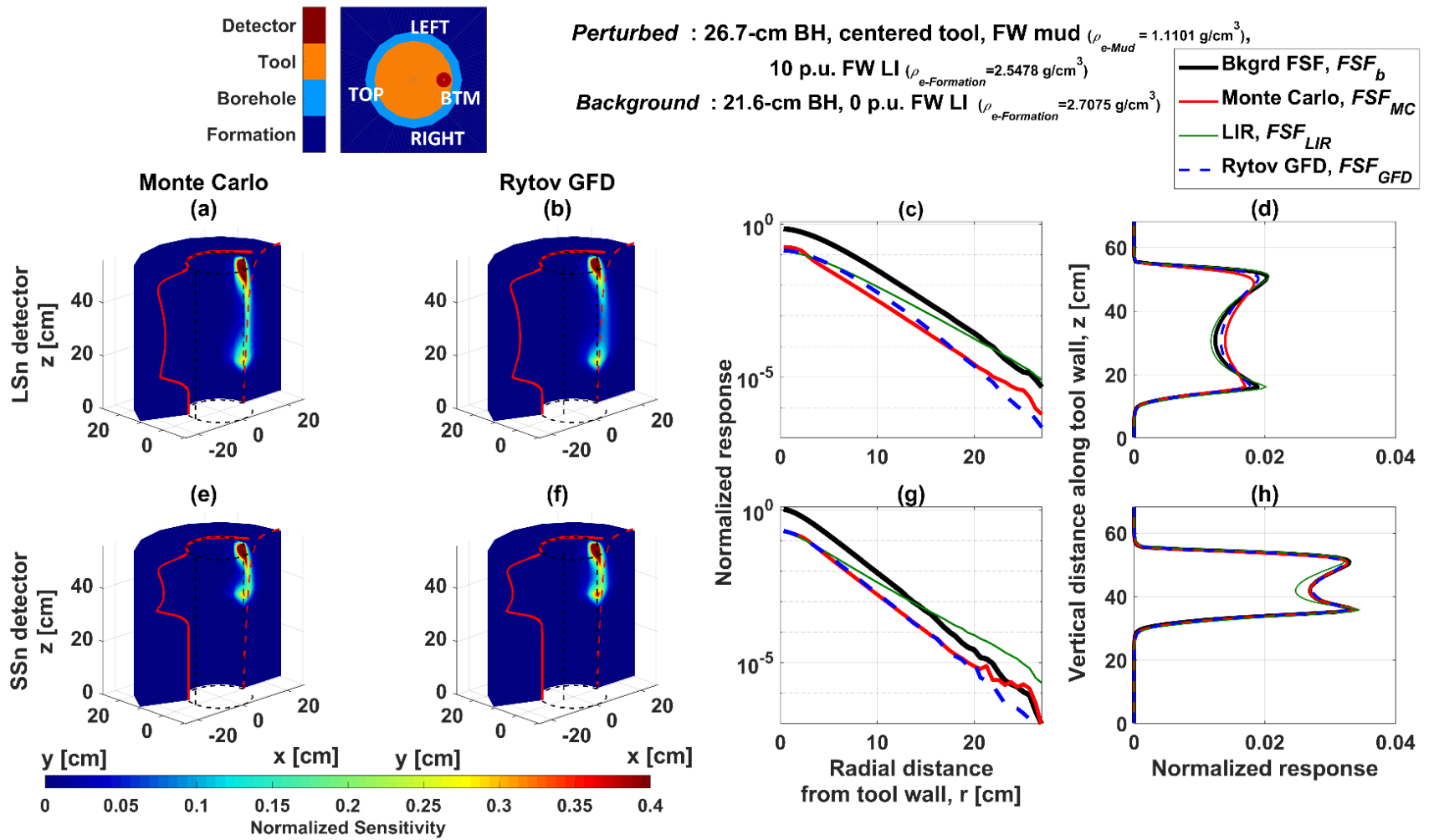


Figure 5.7.

Figure 5.7. Qualitative comparison of LIR, GFD, and MC-derived sensitivity functions for a 26.7-cm (10.5-in) borehole with freshwater mud, in a 10 p.u. freshwater-filled limestone formation. The schematic diagram describes the corresponding borehole/tool configuration. Top and bottom panels show sensitivity functions at long- and short-spaced detectors, respectively. (a)(e) 3D perturbed sensitivity functions calculated with MCNP, FSF_{MC} . The borehole wall is identified with dashed black lines, and solid red lines show 1D radial projection, 1D azimuthal projection, and radial J-factor of the sensitivity functions; (b)(f) 3D perturbed sensitivity functions calculated using gamma flux-difference approximations, FSF_{GFD} . (c)(g) 1D vertical, and (d)(h) 1D radial projections of LIR, GFD, and MC-derived sensitivity functions. The solid black line describes the background sensitivity function, FSF_b , solid red line identifies the perturbed MC-derived FSF, FSF_{MC} , dashed blue line describes the perturbed, FSF_{GFD} , calculated using gamma-ray point kernel approximation. The perturbed FSF_{LIR} , calculated with the LIR algorithm, is shown with a solid green line.

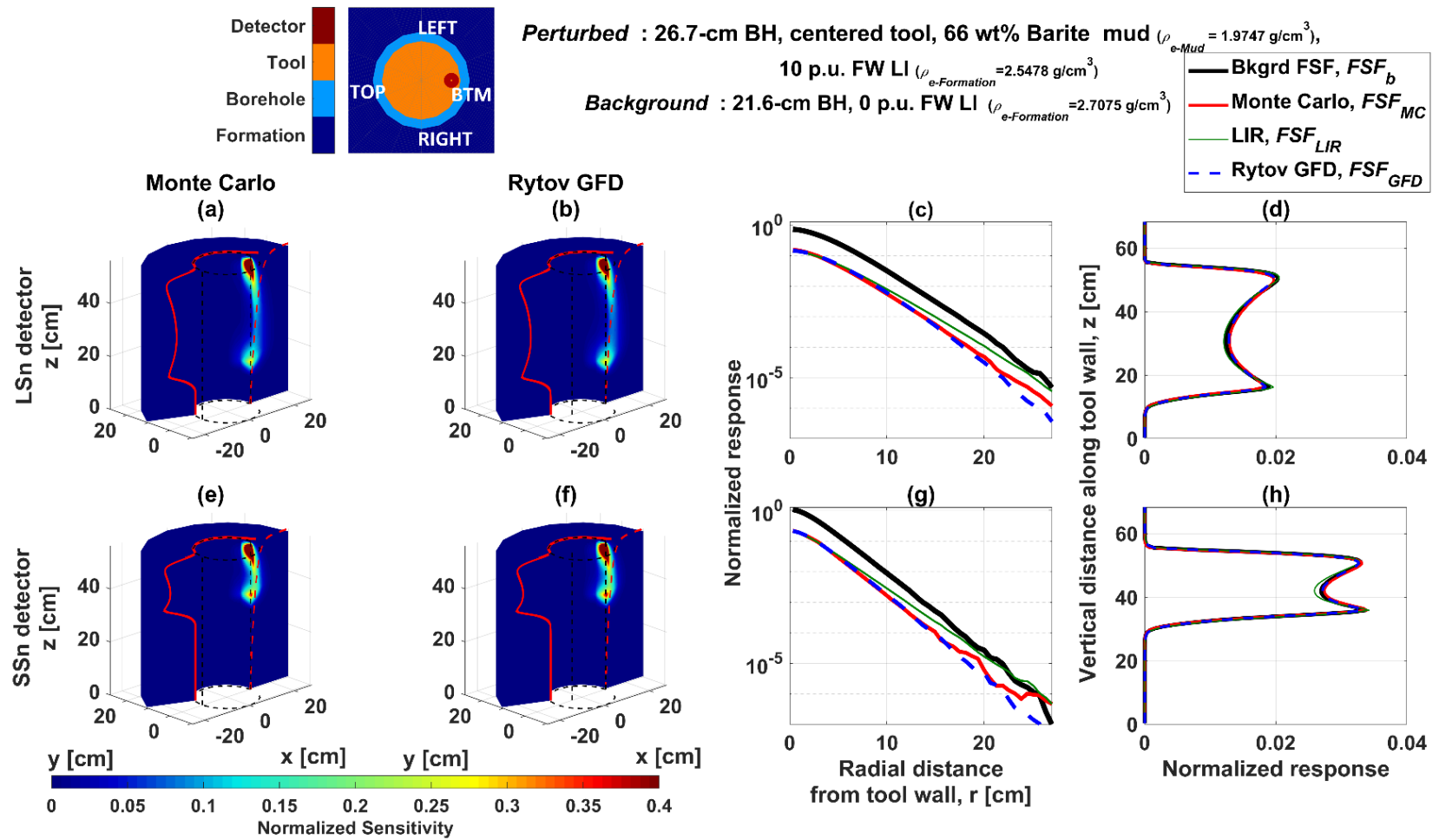


Figure 5.8.

Figure 5.8. Qualitative comparison of LIR, GFD, and MC-derived sensitivity functions for a 26.7-cm (10.5-in) borehole with freshwater mud, in a 10 p.u. freshwater-filled limestone formation. The schematic diagram describes the corresponding borehole/tool configuration. Top and bottom panels show sensitivity functions at long- and short-spaced detectors, respectively. (a)(e) 3D perturbed sensitivity functions calculated with MCNP, FSF_{MC} . The borehole wall is identified by dashed black lines, while solid red lines show 1D radial projection, 1D azimuthal projection, and radial J-factor of the sensitivity functions; (b)(f) 3D perturbed sensitivity functions calculated using gamma flux-difference approximations, FSF_{GFD} . (c)(g) 1D vertical, and (d)(h) 1D radial projections of LIR, GFD, and MC-derived sensitivity functions. The solid black line describes the background sensitivity function, FSF_b , solid red line identifies the perturbed MC-derived FSF, FSF_{MC} , dashed blue line describes the perturbed FSF_{GFD} , calculated using gamma-ray point kernel approximations. The perturbed FSF_{LIR} , calculated with the LIR algorithm is shown with a solid green line.

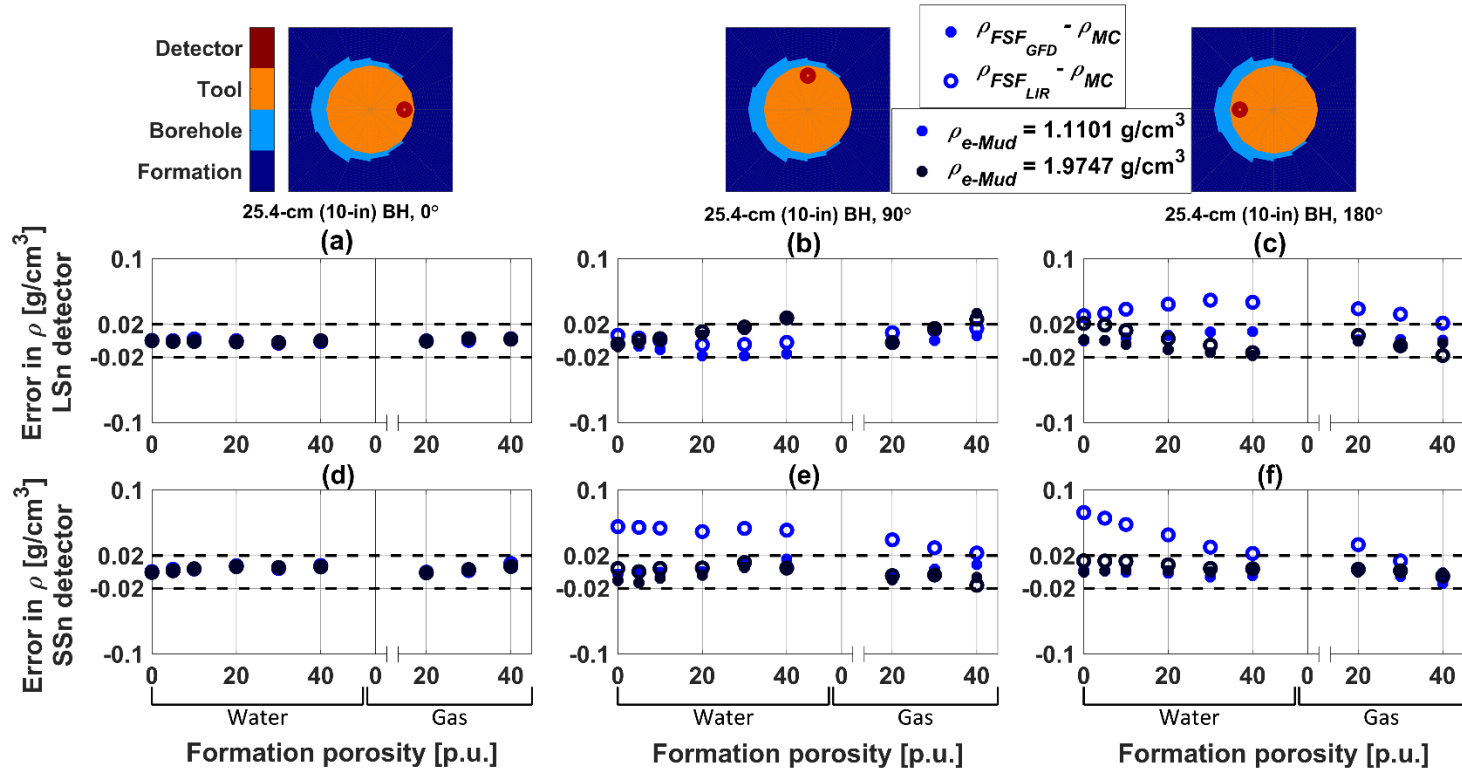


Figure 5.9. Density accuracy at long- (top panels) and short-spaced (bottom panels) detectors in freshwater and gas-filled limestone formations at (a)(d) 0°, (b)(e) 90°, and (c)(f) 180° sector orientation for a 25.4-cm (10-in) borehole (eccentered tool configuration), with borehole mud densities of 1 g/cm³ and 2.0440 g/cm³. Density errors are calculated with respect to densities estimated from MCNP gamma-ray counts, ρ_{MC} . Point and circle markers identify errors for densities calculated using the GFD method, $\rho_{FSF_{GFD}}$, and LIR method, $\rho_{FSF_{LIR}}$, respectively.

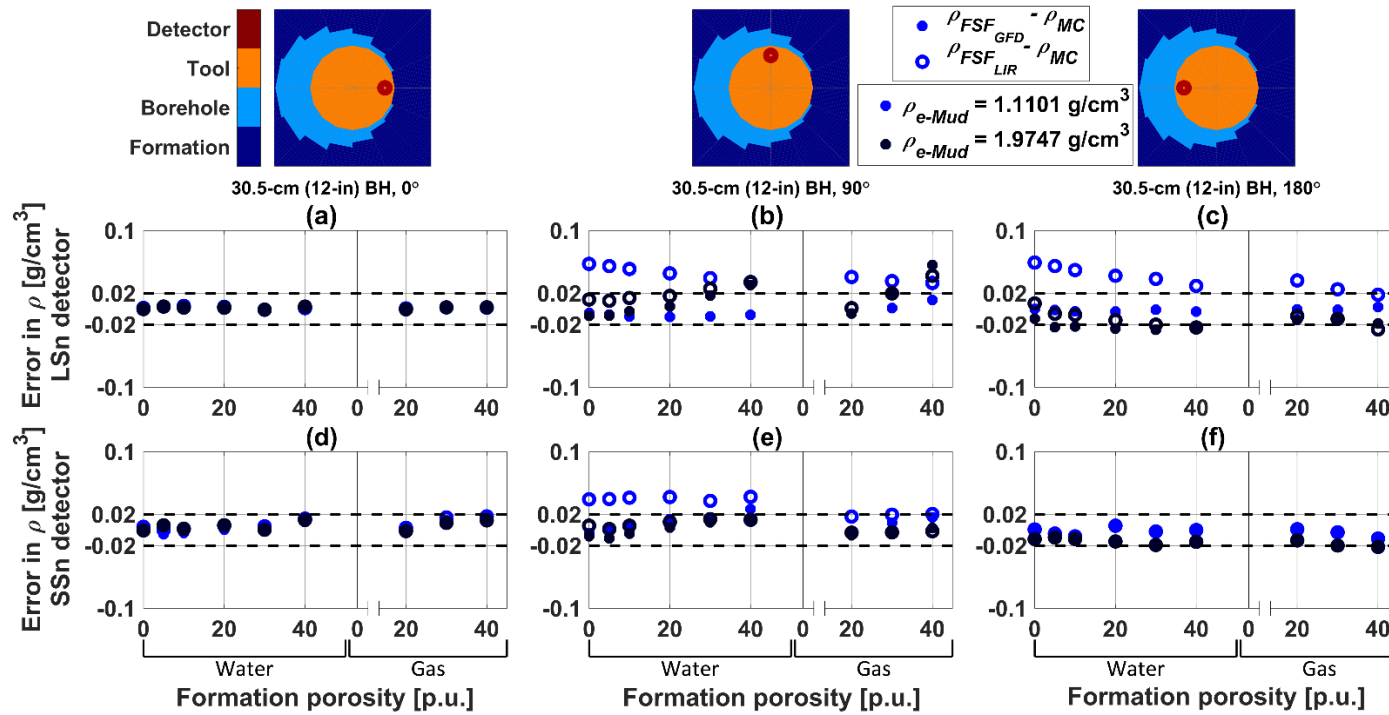


Figure 5.10. Density accuracy at long-spaced (top panels) and short-spaced (bottom panels) detectors in freshwater and gas-filled limestone formations at (a)(d) 0°, (b)(e) 90°, and (c)(f) 180° sector orientation for a 30.5-cm (12-in) borehole (eccentered tool configuration), with borehole mud densities of 1 g/cm³ and 2.0440 g/cm³. Density errors are calculated with respect to densities estimated from MCNP gamma-ray counts, ρ_{MC} . Point and circle markers identify errors for densities calculated using the GFD method, $\rho_{FSF_{GFD}}$, and LIR method, $\rho_{FSF_{LIR}}$, respectively.

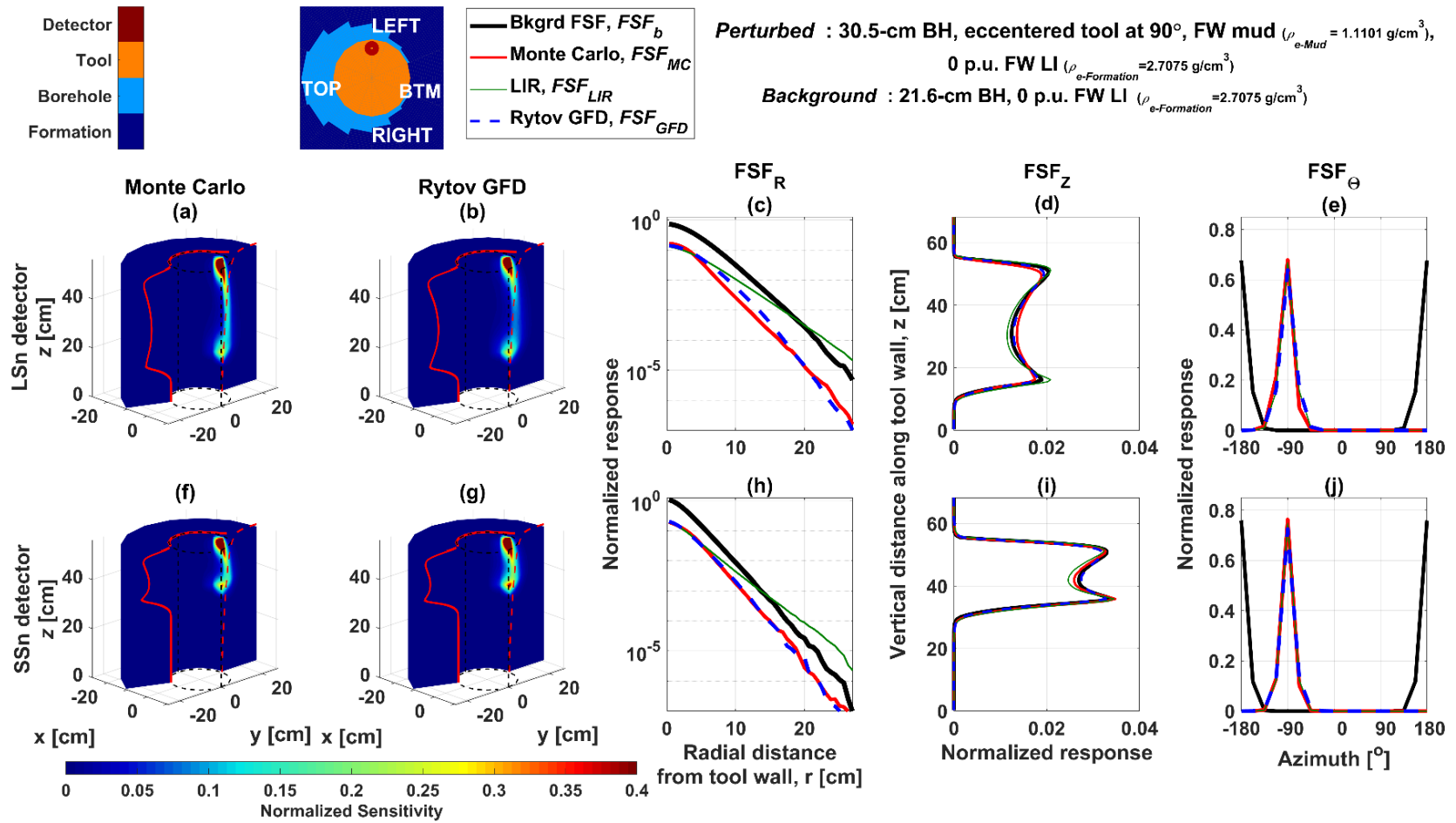


Figure 5.11.

Figure 5.11. Qualitative comparison of LIR, GFD, and MC-derived sensitivity functions for a 30.5-cm (12-in) borehole (eccentered tool configuration) with freshwater mud, in a 0 p.u. freshwater-filled limestone formation at 90° orientation (left sector). The schematic diagram describes the corresponding borehole/tool configuration. Top and bottom panels show sensitivity functions at long- and short-spaced detectors, respectively. (a)(f) 3D perturbed sensitivity function calculated using MCNP, FSF_{MC} . Borehole wall is identified by dashed black lines and solid red lines identify 1D projections of the sensitivity function (radial projection, azimuthal projection, and radial J-factor); (b)(g) 3D perturbed sensitivity function calculated using gamma flux-difference approximations, FSF_{GFD} ; 1D vertical (c)(h), radial (d)(i), and azimuthal (e)(j) projections of sensitivity functions. The solid black line represents the background sensitivity function, FSF_b , solid red line identifies perturbed MC-derived FSF, FSF_{MC} , and the dashed blue line describes the perturbed FSF_{GFD} calculated using gamma-ray point kernel approximations. The perturbed FSF_{LIR} , calculated with the LIR algorithm, is shown with a solid green line.

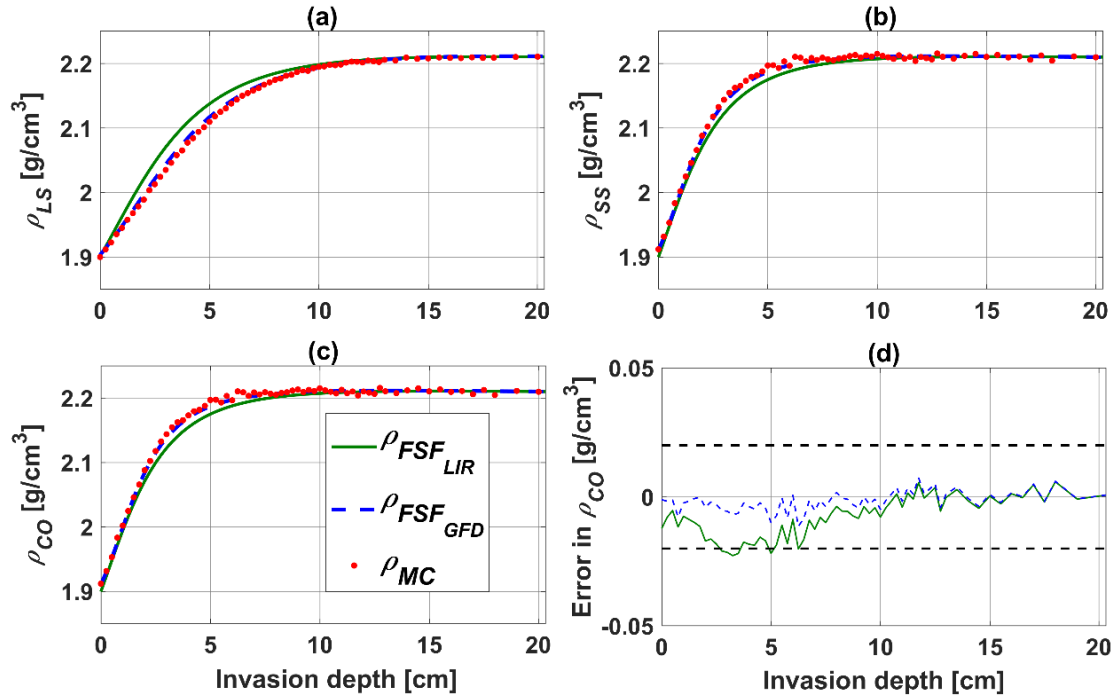


Figure 5.12. Comparison of bulk density simulated with LIR (solid green line), GFD (dashed blue line), and MC (red markers) algorithms for a 30 p.u. gas-filled limestone ($\rho_{b-Formation}=1.9023 \text{ g/cm}^3$) invaded with freshwater mud ($\rho_{b-Mud}=1.0 \text{ g/cm}^3$). (a) Bulk density at the long-spaced gamma-ray detector, (b) at the short-spaced gamma-ray detector, and (c) compensated density versus invasion depth. (d) Error in simulated density with respect to MC-derived density.

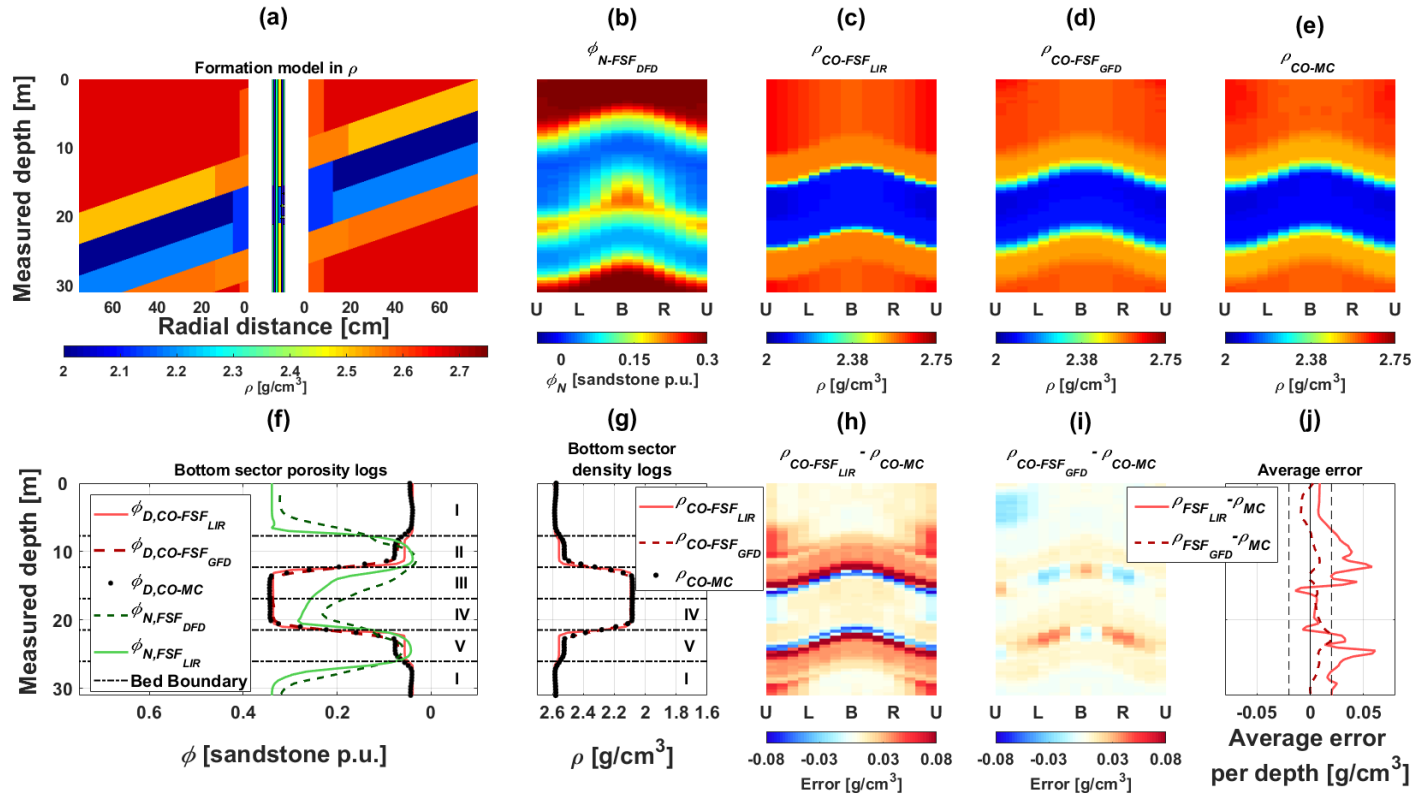


Figure 5.13. Synthetic case with approximate "teardrop" invasion profile. (a) Description of the layered earth model in bulk density (not to scale); (b) borehole image of neutron porosity simulated using diffusion flux-difference approximations; comparison of borehole image for simulated compensated density calculated using (c) sensitivity functions derived from the LIR algorithm, (d) sensitivity functions computed using gamma flux-difference approximations, and (e) MCNP counts; (f) bottom-sector porosity logs (layers properties listed in **Table 5.2**), and (g) density logs; residuals of compensated density simulated using (h) LIR, and (i) GFD algorithms with respect to density derived from MCNP counts; (j) average error per depth.

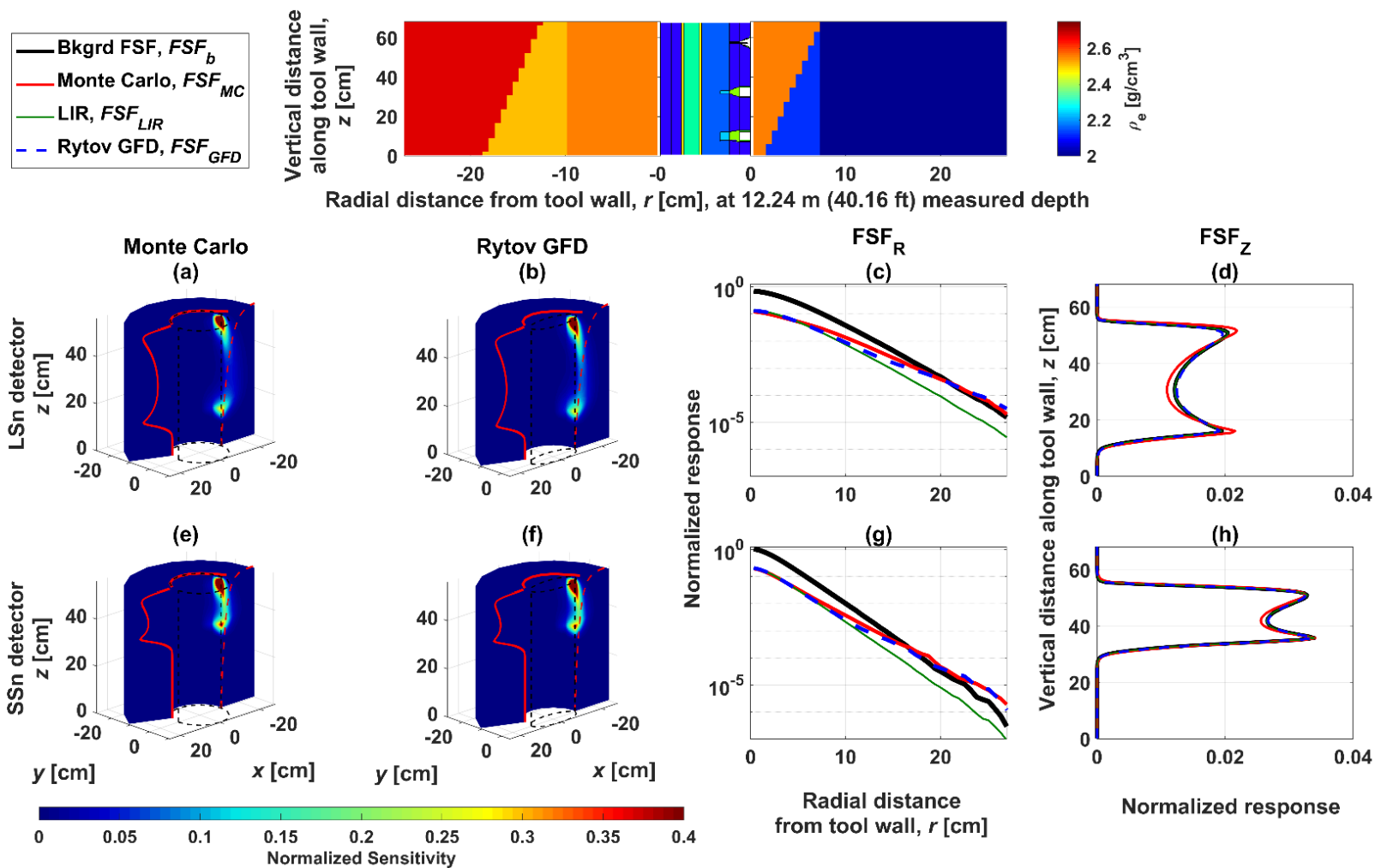


Figure 5.14.

Figure 5.14. Qualitative comparison of LIR, GFD, and MC-derived sensitivity functions for the synthetic case with an approximate “teardrop” invasion profile, at measured depth 12.2 m (40.16 ft), at the bottom sector. The schematic diagram describes the corresponding borehole/tool configuration. Top and bottom panels show sensitivity functions at long- and short-spaced detectors, respectively. (a)(e) 3D perturbed sensitivity functions calculated with MCNP, FSF_{MC} . The borehole wall is identified by dashed black lines, and solid red lines show 1D radial projection, 1D azimuthal projection, and radial J-factor of the sensitivity functions; (b)(f) 3D perturbed sensitivity functions calculated using gamma flux-difference approximations, FSF_{GFD} . (c)(g) 1D vertical, and (d)(h) 1D radial projections of LIR, GFD, and MC-derived sensitivity functions. The solid black line identifies the background sensitivity function, FSF_b , solid red line identifies perturbed MC-derived FSF, FSF_{MC} , dashed blue line describes the perturbed FSF_{GFD} , calculated using gamma-ray point kernel approximations. The perturbed FSF_{LIR} , calculated with the LIR algorithm, is shown as a solid green line.

Chapter 6: Summary, Conclusions, and Recommendations

This chapter contains a summary of the dissertation, gives important conclusions stemming from my research, and provides recommendations for future studies.

6.1 SUMMARY

The objectives of this dissertation were the following:

- (1) To develop a Neutron-Gamma density measurement method with similar accuracy than measurements obtained using Gamma-Gamma density instruments.
- (2) To develop alternative Neutron-Gamma density measurement interpretation methods based on rapid numerical simulations for cases where conventional interpretation algorithms yield inaccurate results.
- (3) To develop rapid forward modeling algorithms to accurately simulate and mitigate borehole environmental effects for neutron and density porosity measurements.

In the first technical section of this dissertation, I designed a theoretical, albeit realistic logging-while-drilling (LWD) Neutron-Gamma density tool to accurately measure bulk density without using a chemical source. I examined the measurement physics and determined that the tool design should include two gamma-ray and two fast neutron detectors to deliver density accuracy that favorably compares with that of Gamma-Gamma density measurements. It was

shown that Neutron-Gamma density measurements are affected by three-dimensional (3D) geometrical and borehole effects that complicate petrophysical interpretation by masking true formation properties. Therefore, I also developed a fast-forward algorithm based on first-order Taylor series expansions to improve petrophysical analysis across spatially complex geometries.

One of the limitations of Neutron-Gamma density is its sensitivity to borehole environmental effects. First-order fast numerical simulations can improve interpretation when standoff is less than 1.27 cm (0.5 in). However, for larger values of standoff, sensitivity flux perturbations introduce higher-order effects whereby Neutron-Gamma density measurements can no longer be modeled accurately using first-order approximations. Therefore, I introduced new methods to simulate borehole nuclear measurements in enlarged boreholes. For neutron porosity measurements, diffusion flux-difference (DFD) approximations are coupled with a new two-step algorithm that yields 1 porosity unit (p.u.) error on average when compared with Monte Carlo simulations. At boundaries between beds exhibiting large contrasts in electron density, Gamma-Gamma density measurements respond to higher-order effects because of sensitivity flux perturbations. I introduced a new method, referred to as gamma flux-difference (GFD), to quantify such flux perturbations using gamma-ray point kernel approximations, and I developed a fast-forward modeling algorithm yielding maximum density errors of 0.02 g/cm³ in enlarged boreholes.

6.2 CONCLUSIONS

The most important conclusions stemming this research are summarized below, by chapter.

6.2.1 Chapter 1: Physics, Applications, and Limitations of Borehole Neutron-Gamma Density Measurements

- I designed a theoretical, albeit realistic LWD Neutron-Gamma density tool in MCNP (the Monte Carlo N-Particle code, Goorley, 2014). Two fast neutron detectors are required to capture the variability of the neutron-induced secondary gamma-ray source (in space, energy, and intensity) and measure bulk density with an accuracy that favorably compares with that of Gamma-Gamma density measurements in formations with complex mineralogy. With this design, the accuracy of the density estimation algorithm is 0.012 g/cm³ in clean formations and 0.019 g/cm³ in shales and shaly formations. Such accuracies represent an improvement of 50% as compared to those reported in other publications.
- The main advantage of Neutron-Gamma density is that it eliminates radioactive chemical sources, thus reducing the risks and costs associated with operating, handling, and transporting chemical sources. Another advantage is that Neutron-Gamma density is less affected by mud-filtrate invasion because its depth of investigation is twice as large as that of Gamma-Gamma density measurements.
- The main limitation of Neutron-Gamma density is the measurement's sensitivity to borehole environmental effects. Because the measurement is uncompensated, borehole environmental effects

are mitigated using empirical corrections. However, such corrections require a-priori knowledge of standoff and mud type. Additionally, I showed that they should be avoided when standoff is greater than 0.64 cm (0.25 in) as they are no longer independent of formation properties. Additional limitations are that Neutron-Gamma density measurements have relatively low vertical resolution (76 cm) and deliver asymmetrical log responses at boundaries between beds with large contrasts in hydrogen index and/or bulk density. Therefore, other well logs should be used to identify bed boundaries and petrophysical interpretation practices should be adapted to account for the relatively low vertical resolution of the measurement.

6.2.2 Chapter 2: Rapid Forward Modeling of Borehole Logging-While-Drilling Neutron-Gamma Density Measurements

- Forward modeling algorithms were developed to rapidly and accurately simulate Neutron-Gamma density measurements using first-order perturbation theory coupled with flux sensitivity functions (FSFs). The earth model is described with new characteristic cross sections, also referred to as perturbation parameters, whose variations govern that of the detector counts. The primary advances of the fast-forward model include:
 - Perturbation parameters are defined by combining the average macroscopic elastic and absorption cross sections, hydrogen content index, bulk density, and electron density such that they yield a one-to-one correspondence with particle counts at each detector. The average macroscopic elastic and

absorption cross sections are calculated assuming neutron transport in a strongly absorbing and purely scattering medium. Further, hydrogen content index is a new parameter that is linearly correlated with hydrogen index.

- For each detector, sensitivity functions are pre-computed using MCNP and stored in a library for future use. They are organized according to the fast slowing-down length because variations in this parameter are linearly correlated with those of the flux sensitivity functions across homogeneous formations. The fast slowing-down length, which is calculated using a modified version of Kreft's method, approximates the distance travelled by fast neutrons from their point of origin at 14.1 MeV to the location where they fall below fast energy levels (1 MeV).
- At each measured depth, sensitivity functions are selected using the linear iterative refinement (LIR) method, which performs iterative linear interpolations between base-case FSFs. In highly perturbed models, such as enlarged boreholes, first-order approximations become inaccurate because perturbations in the sensitivity flux give rise to higher-order effects. Although maximum density errors are below 0.02 g/cm^3 up to 1.27-cm (0.5-in) standoff in homogeneous formations, the accuracy of the simulated bulk density is degraded to 0.04 g/cm^3 when standoff is 2.54-cm (1-in).

- Benchmark simulations in complex logging environments showed that the first-order fast-forward algorithm achieves sufficient speed and accuracy to be combined with inversion-based interpretation. Across thinly-bedded, dipping or invaded formations, formations with complex mineralogy, and when standoff is less than 1.27-cm (0.5-in), the algorithm delivers root-mean-square errors of up to 0.023 g/cm³, maximum errors (at the 90-th percentile) of up to 0.035 g/cm³, and is 500,000 times faster than MCNP.

6.2.3 Chapter 3: Improvements of Fast Modeling of LWD Neutron Logs in Enlarged Boreholes for a Commercial LWD Tool from Service Provider Baker Hughes

- Rapid numerical simulations of neutron measurements that rely on diffusion flux-difference approximations may yield inaccurate neutron porosity results in enlarged boreholes when compared with the neutron porosity calculated using MCNP detector counts. Coupled with the DFD method, I introduced a two-step algorithm based on sensitivity function base cases and count base cases to minimize the size of the borehole perturbations, thus increasing the validity of the Taylor series expansion. The algorithm was developed for an LWD neutron tool from service provider Baker Hughes, a GE company.
- Benchmark simulations against MCNP for enlarged boreholes, and for synthetic examples, showed that the two-step algorithm yields average errors of 1 p.u. and maximum errors of 2 p.u. when compared to Monte Carlo simulations.

6.2.4 Chapter 4: Fast Modeling of Gamma-Gamma Density Measurements via Gamma-Ray Point Kernel Approximations

- Across regions with properties that contrast significantly, for example in the presence of enlarged boreholes, Gamma-Gamma density measurements respond to higher-order effects in the form of sensitivity flux perturbations. Fast-forward modeling algorithms based on first-order approximations, such as the LIR method, do not accurately simulate Gamma-Gamma density measurements in such conditions.
- I developed a new method to accurately and rapidly simulate Gamma-Gamma density measurements in enlarged boreholes. The gamma flux-difference method uses an exponential gamma-ray point kernel model, with corrections for buildup and standoff heterogeneity effects, coupled with a Rytov approximation to quantify three-dimensional spatial sensitivity flux perturbations.
- Empirical correction coefficients account for both the presence of spatial heterogeneities resulting from standoff and for flux buildup. They vary with detector position, standoff, and the mud density in the borehole, but are independent of formation rock composition. I developed two-dimensional (2D) interpolation maps to compute the correction coefficients for arbitrary combinations of mud density and standoff.
- Extensive benchmarking against MCNP showed that the GFD algorithm delivers bulk density errors below 0.03 g/cm^3 in spatially complex geometries, which include formations with complex

mineralogy, high-angle/horizontal wells, thinly-bedded or invaded formations, and enlarged boreholes. Density accuracy is 0.02 g/cm^3 with standoff up to 4.45-cm (1.75-in) in homogeneous formations. Compared with the LIR method, average density accuracy is improved by up to 0.045 g/cm^3 in invaded high-angle/horizontal wells and 0.1 g/cm^3 in enlarged boreholes. Note that density errors are calculated with respect to the bulk density calculated from MCNP detector counts.

6.3 RECOMMENDATIONS

Because of the lack of available field measurements, the research topics documented in this dissertation are based on Monte Carlo modeling. While MCNP accurately simulates borehole nuclear measurements, the work in this dissertation would nonetheless benefit from comparison with laboratory and/or field measurements.

- The Monte Carlo modeling assumptions implemented when designing fast neutron and gamma-ray detectors for the Longhorn Neutron-Gamma density tool could be evaluated against laboratory or test-pit measurements.
 - Particle counts simulated with MCNP using Helium-4 detectors could be compared with laboratory measurements to validate the Monte Carlo modeling assumptions and ensure proper calibration. The efficiency of zinc-sulfide (ZnS) and

Helium-4 detectors could also be compared using laboratory measurements.

- Non-capture gamma-ray counts are simulated using a lower energy cutoff that “kills” neutrons below 1 MeV. Field interpretation procedures are more complex in that they involve subtracting the early capture spectrum from the burst spectrum. I recommend benchmarking and calibrating Monte Carlo simulated gamma-ray counts against inelastic gamma-ray counts measured in test pits.
- The Longhorn Neutron-Gamma density tool includes two gamma-ray scintillators and two fast neutron detectors that deliver one density measurement with accuracy comparable to that of Gamma-Gamma density measurements. A third gamma-ray scintillator could be introduced to deliver two density measurements instead of one, such that “spine and rib” compensation can be implemented. For example, a recent wireline logging tool (Rose et al., 2015) makes use of a yttrium aluminum perovskite (YAP) scintillator to measure gamma-ray counts at distances greater than that of long-spaced detectors.
- Inversion-based interpretation of Neutron-Gamma density measurements could be developed using the first-order fast-forward modeling algorithm for the Longhorn Neutron-Gamma density tool. Synthetic data generated with the first-order modeling algorithm could be used for partial benchmarking, however field measurements would be required to deliver a complete (and compelling) validation.

- I recommend that the DFD two-step algorithm be implemented with inversion procedures to simplify and automate the petrophysical interpretation process. Inversion-based interpretation could then be applied to field examples acquired with the Baker Hughes LWD neutron-porosity logging tool.
- I suggest developing inversion-based borehole environmental corrections for neutron porosity and Gamma-Gamma density measurements using the DFD two-step and gamma flux-difference fast-forward modeling algorithms, respectively. The interpretation results could be compared with those obtained using the “spine and rib” and dual spacing compensation procedures.
- The GFD algorithm was developed to simulate and mitigate borehole environmental effects for Gamma-Gamma density measurements by quantifying flux perturbations arising at the borehole wall. The DFD two-step algorithm achieves similar results with neutron measurements. Higher-order effects also occur in measurements based on two-particle transport, for which borehole environmental corrections using compensation algorithms can be impractical. For example, the first-order forward model for Neutron-Gamma density yields inaccurate results for standoff values greater than 1.27 cm (0.5 in). Therefore, I recommend combining the methods employed by the GFD and DFD algorithms to develop higher-order numerical simulations for measurements based on coupled neutron and gamma-ray transport. To quantify sensitivity flux perturbations at gamma-ray detectors, I propose two possible approaches:

(1) The first approach would involve sequentially implementing the DFD and GFD methods. At gamma-ray detectors, flux perturbations resulting from fast neutron transport can be quantified using the diffusion flux-difference model, where transport correction coefficients are derived from the flux-fitting procedure applied at fast neutron detectors. A diffusion flux-difference sensitivity function (FSF_{DFD}) is computed with respect to MC-derived base-case FSFs and accounts for flux perturbations caused by variations in the secondary gamma-ray source. Then, the perturbed FSF_{DFD} is regarded as a distributed source to implement the gamma-ray point kernel approximation and derive the gamma flux-difference distributed function.

(2) In the second approach, a coupled flux-difference function based on couple-field theory (Stevens and Trubey, 1972; Zhang et al., 2017) could be derived. Coupled neutron and gamma-ray transport would be approximated with a single equation, whose solution would give rise to coupled Green's function kernels. Because the equations involved are more complex, additional assumptions would be required, for example, regarding the spatial distribution of the fast neutron flux.

Appendix: Density Accuracy Using an Estimation Algorithm Based on One Fast Neutron and Two Inelastic Gamma-Ray Detectors

Zhang et al. (2017) developed a Neutron-Gamma density estimation algorithm based on coupled field theory and MCNP modeling. They used simplifying assumptions to derive the relationship

$$\rho_b = c_1 \cdot \log_e \left(\frac{GRLS}{GRSS} \right) + c_2 \cdot \log_e (FastN) + c_3, \quad (A.1)$$

where ρ_b is material bulk density, and c_1 , c_2 , and c_3 are fitting coefficients derived from MCNP modeling; $GRLS$ designates gamma-ray counts at the long-spaced gamma detector, and $GRSS$ at the short-spaced gamma detector. $FastN$ designates neutron counts at the near fast neutron detector.

Fitting coefficients c_1 , c_2 , and c_3 can also be determined by solving the linear inverse problem $\mathbf{P}\mathbf{w}=\mathbf{q}$, with

$$\mathbf{P} = \begin{bmatrix} \log_e \left(\frac{GRLS_1}{GRSS_1} \right) & \log_e (FastN_1) & 1 \\ \vdots & \vdots & \vdots \\ \log_e \left(\frac{GRLS_k}{GRSS_k} \right) & \log_e (FastN_k) & 1 \\ \vdots & \vdots & \vdots \\ \log_e \left(\frac{GRLS_{ktot}}{GRSS_{ktot}} \right) & \log_e (FastN_{ktot}) & 1 \end{bmatrix}, \quad (A.2)$$

$$\mathbf{w} = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}, \quad (\text{A.3})$$

and

$$\mathbf{q} = \begin{bmatrix} \rho_{b,1} \\ \vdots \\ \rho_{b,k} \\ \vdots \\ \rho_{b,ktot} \end{bmatrix}, \quad (\text{A.4})$$

where gamma-ray and neutron counts are computed in *ktot* formations of different bulk density, $\rho_{b,k}$. **Table A.1** lists the coefficients c_1 , c_2 , and c_3 for the Longhorn Neutron-Gamma density tool, and **Figure A.1** shows a cross-plot of bulk density calculated using the density estimation algorithm developed by Zhang et al. (equation A.1), and formation bulk density, across diverse solid and fluid rock compositions. The algorithm described in equation A.1 provides high density accuracies in clean formations (0.015 g/cm³) but performs poorly in anhydrite (0.1 g/cm³ accuracy), and in shale and shaly formations (0.05 g/cm³ accuracy), especially at low porosities (**Figure A.2**).

Fitting coefficient	Value
c_1	0.9219
c_2	0.5776
c_3	5.2206

Table A.1. Fitting coefficients of the Longhorn Neutron-Gamma density tool for the density estimation algorithm (equation A.1) developed by Zhang et al. (2017).

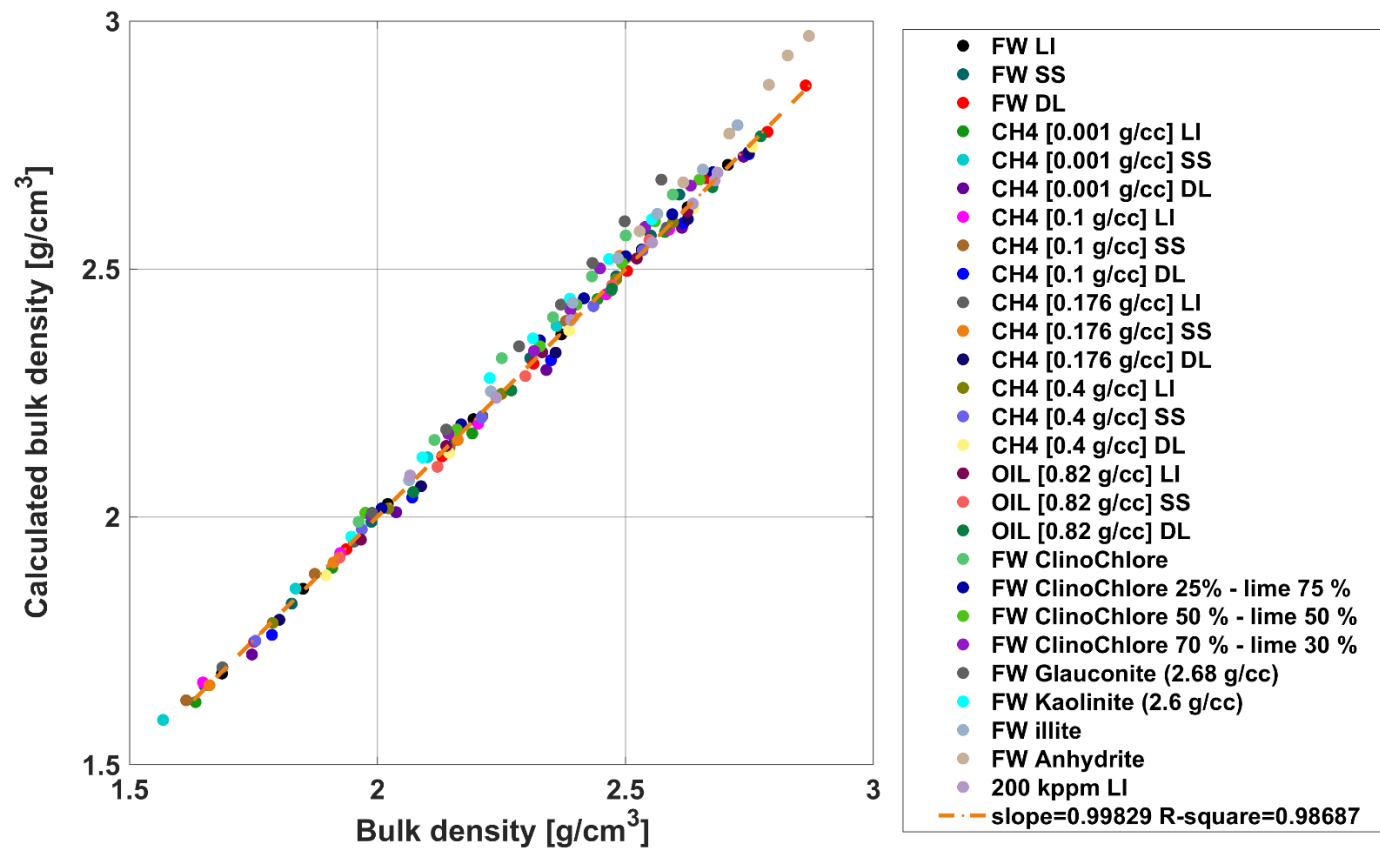


Figure A.1. Cross-plot of bulk density calculated with the density estimation algorithm developed by Zhang et al. (2017) using equation A.1, and formation bulk density across diverse solid and fluid rock compositions. FW stands for “freshwater-filled”, 200 kppm stands for “formation filled with 200 kppm NaCl water”.

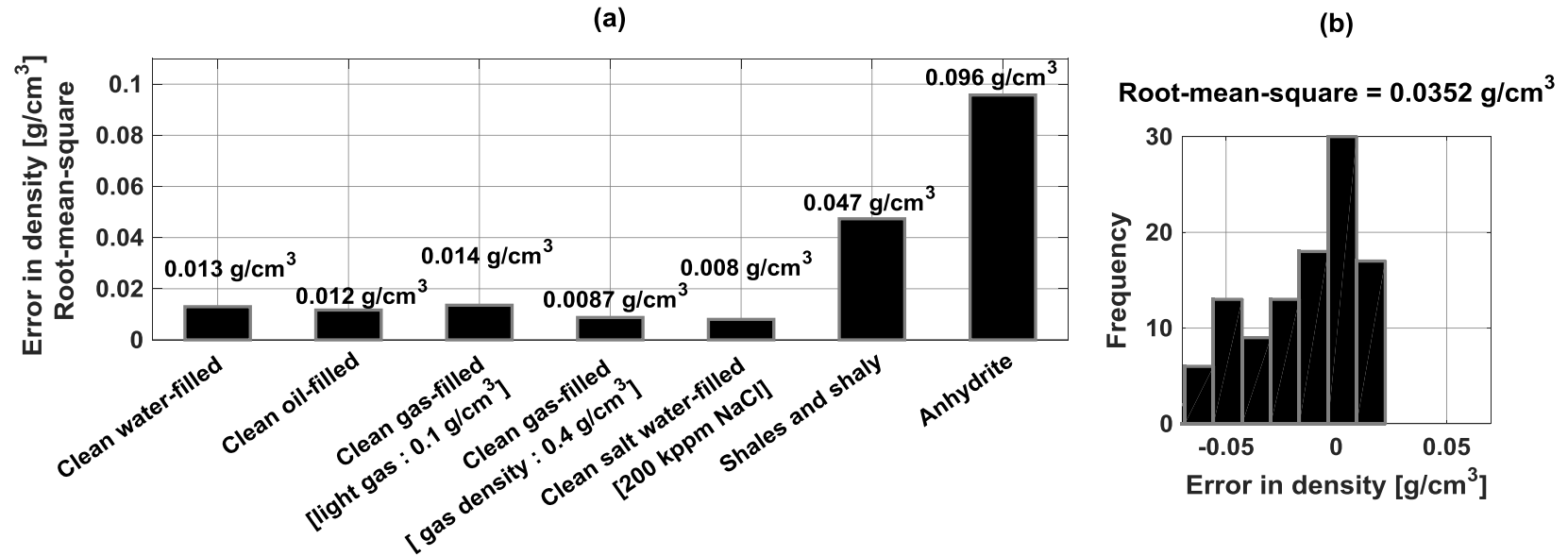


Figure A.2. (a) Root-mean-square error for densities calculated with the density estimation algorithm developed by Zhang et al. (2017) using equation A.1 across seven types of rock compositions, and (b) overall density accuracy. RMS stands for root-mean-square.

List of Symbols

General

A	Forward operator matrix
A	Atomic mass
A_1	Parameter for the single-term Taylor form of the buildup factor
a	Fitting coefficients for the density estimation algorithm
α	Modified cross section parameter [1/cm]
α_1	Parameter for the single-term Taylor form of the buildup factor
B	Buildup factor
b	Observed data vector
c	Fitting coefficients for the perturbation parameters
d	Deuteron
E	Energy of scattered particles [eV]
E'	Energy of incoming particles [eV]
ε	Arbitrarily small positive quantity
F	Nonlinear forward operator
$Fast$	Fast neutron detector counts [Counts/SP]
$FastN$	Near fast neutron detector counts [Counts/SP]
$FastF$	Far fast neutron detector counts [Counts/SP]
Fp	Perturbation parameter
G	Gamma-ray point kernel
Gfd	Gamma-ray flux-difference distributed function

GR	Gamma-ray detector counts
$GRLS$	Non-capture gamma-ray counts at the long-spaced gamma detector [Counts/SP]
$GRSS$	Non-capture gamma-ray counts at the short-spaced gamma detector [Counts/SP]
Γ	Distributed point kernel gamma-ray flux
η	Correction coefficient
θ	Azimuthal angle [°]
J	Derivative of the distributed point kernel gamma-ray flux
k	Fitting coefficients for the perturbation parameters
L, ℓ	Distances [cm]
L'_{1E}	Modified travel length [cm]
L_{Fast}	Fast slowing-down length (to 1 MeV) [cm]
L_m	Migration length [cm]
L_s	Slowing-down length (to thermal energy levels) [cm]
m	m-th order
M	Molecular weight [g/mol]
m_1	Fitting coefficient for the density estimation algorithm
μ	Linear attenuation coefficient [1/cm]
μ'	Effective linear attenuation coefficient [1/cm]
μ_{Co}	Compton linear attenuation coefficient per atom [1/cm]
μ_m	Mass attenuation coefficient [cm ² /g]
μ_{m-To}	Total mass attenuation coefficient [cm ² /g]
μ_{m-Co}	Compton mass attenuation coefficient per atom [cm ² /g]
μ_{m-Pa}	Pair production mass attenuation coefficient [cm ² /g]

μ_{m-Ph}	Photoelectric mass attenuation coefficient [cm^2/g]
μ_s	Macroscopic scattering cross section [$1/\text{cm}$]
μ_{To}	Total linear attenuation coefficient or total macroscopic cross section [$1/\text{cm}$]
N	Detector response [$\text{particles}/\text{cm}^2\text{-sec}$]
n	Neutron
N_{Av}	Avogadro's number
N_d	Number density [cm^{-3}]
ν	Number of atoms
ξ	Average logarithmic energy decrement []
$\mathbf{P}$	Forward operator matrix
p	Proton
$\mathbf{q}$	Observed data vector
$\mathbf{r}$	Position vector in 3D space
r	Radial direction [cm]
ρ_e	Electron density [mol/cm^3]
ρ_b	Bulk density [g/cm^3]
S	Particles source or source strength [$\text{particles}/\text{cm}^3\text{- sec - steradian - eV}$]
S_0	Isotropic monoenergetic point source [$\text{particles}/\text{sec}$]
Σ	Macroscopic energy cross-section [cm^{-1}]
σ	Microscopic energy cross-section [barn]
${}_e\sigma_{Co}$	Compton scattering microscopic cross section per electron [barn]
V	Volumetric concentration
ϕ_N	Neutron near-to-far ratio porosity [p.u.]

Ψ	Angular flux at $\mathbf{r}$ of energy E and direction Ω [particles/cm ² -steradian-eV]
ψ	Scalar flux function at $\mathbf{r}$ [particles/cm ² -sec]
ψ_{GR}	Gamma-ray flux [particles/cm ²]
ψ_i	Initial flux [particles/cm ²]
$\mathbf{w}$	Model parameter vector
x	One particle (such as neutron, n , proton, p , deuteron, d , or alpha, α) or a combination of particles
$\mathbf{y}$	Model parameter vector
y_{abst}	Elemental absolute yield
Z	Atomic number
z	Vertical direction [cm]
ZJ	Vertical geometrical factor
Ω	Unit direction of scattered particles []
Ω'	Unit direction of incoming particles []

Subscripts, Superscripts, and Operators

a	Thermal-neutron absorption
abs	Absorption
$abst$	Absolute
b	Base-case or background
$b-C$	Count base-case
$b-FSF$	Flux sensitivity function base-case
bd	Boundary
Co	Compton
CO	Compensated

<i>eff</i>	Effective
<i>elastic</i>	Elastic scattering
<i>EM</i>	Earth model
<i>GFD</i>	Gamma flux-difference
<i>het</i>	Heterogeneous
<i>i</i>	Fitting coefficient index
<i>ielt</i>	Element index
<i>itot</i>	Total number of fitting coefficients
<i>j</i>	Mineral or fluid index
<i>k</i>	Formation index
<i>ktot</i>	Total number of formations
<i>lb</i>	Lower-bound
<i>LS</i>	Long-spaced
<i>m</i>	m^{th} -order Taylor's series term
<i>mixt</i>	Mixture
<i>Pa</i>	Pair production
<i>Ph</i>	Photoelectric
<i>R</i>	Observation point (detector)
<i>S</i>	Source point
<i>SS</i>	Short-spaced
<i>To</i>	Total
<i>ub</i>	Upper-bound
<i>updated</i>	Updated
°	Uncollided
—	Average

Acronyms

DFD	Diffusion flux-difference
DL	Dolomite
FastN	Near fast neutron detector (Neutron-Gamma density tool)
FastF	Far fast neutron detector (Neutron-Gamma density tool)
FF	Fast-forward
FFM	Fast-forward numerical simulation model
FSF	Flux Sensitivity Function
FW	Freshwater
GFD	Gamma flux-difference
GGD	Gamma-Gamma density
GRLS	Long-spaced gamma-ray detector (Neutron-Gamma density tool)
GRSS	Short-spaced gamma-ray detector (Neutron-Gamma density tool)
HA/HZ	High-angle/horizontal wells
HI	Hydrogen index
LI	Limestone
LIR	Linear Iterative Refinement
LSn	Long-spaced gamma-ray detector (Gamma-Gamma density tool)
LWD	Logging-while-drilling
MC	Monte Carlo
MCNP	Monte Carlo N-Particle transport
NGD	Neutron-Gamma density
PNG	Pulsed Neutron Generator
p.u.	Porosity unit
RMS	Root-mean-square

SS	Sandstone
SSn	Short-spaced gamma-ray detector (Gamma-Gamma density tool)
SP	Source particle
TST	True stratigraphic thickness
UTNuPRO	University of Texas nuclear parameter calculation program

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