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Status of development of gamma-ray detector response function code or GAMDRF

Fusheng Li*, Xiaogang Han

Baker Hughes, 2001 Rankin Rd, Houston TX 77073, USA

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ABSTRACT

The need for an accurate representation of the detector response functions (DRFs) for sodium iodide (NaI), bismuth germinate (BGO), etc., arises in the oilwell logging business, especially important for spectral logging tools such as a geochemical logging tool. While Monte Carlo models predict the photon spectra incidents on these detectors, the DRFs are used to generate the pulse-height spectra. A Monte Carlo-based γ-ray detector response function code (GAMDRF) was developed to meet the requirements based on complete photon physics.

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1. Introduction

Currently, NaI, BGO, and $LaBr_3$ (Ce) detectors are widely used in nuclear oil logging applications. Detector responses to photon energy ranging from zero up to 10 MeV or higher are extremely important for the prompt γ-ray neutron activation elemental analysis on the subsurface formation rock (e.g., Baker Hughes Formation Lithology Explorer™ (FLeX™)) or the Spectralog tool to determine the natural radiation from three radioisotopes potassium, uranium, and thorium present in the formation rock. Detector response functions are becoming more and more useful in radiation detection for spectrometry purposes because it provides a powerful variance reduction technique. While Monte Carlo models are used to predict the photon spectrum incident on the detectors' surface, the detector response functions are applied to translate incident photons' surface flux spectrum to a pulse-height spectrum.

Large amounts of research efforts have focused on this subject using the experimental method, Monte Carlo, and semi-empirical models. In 1957, Heath published the first edition of a comprehensive γ-ray spectrum catalog and the second edition catalog in 1964 (Heath, 1957, 1964). These documents provide a collection of experimental X-ray and γ-Ray spectra obtained with NaI(Tl) scintillation spectrometers for general laboratory use in the analysis of γ-ray spectra. Later, he published the γ-ray spectrum catalog for Ge(Li) and Si(Li) detectors (Heath, 1974). The Center for Engineering Applications of Radioisotopes (CEAR) at North Carolina State University has a long history of research on detector response functions.

A series of papers (Gardner et al., 1986; Jin et al., 1986; Yacout et al., 1986; He et al., 1990) identified three basic approaches to obtaining detector response functions: an experimental approach, Monte Carlo models, and a semi-empirical method. The experimental approach can be applied directly and was demonstrated in the γ-ray spectrum catalogs by Heath. The disadvantage of this approach is that it requires a large number of difficult experimental measurements under standard conditions and is limited to those factors that affect the detector response functions such as detector dimensions, source-detector-distance, and detector-collimator configuration. Gardner et al., outlined the semi-empirical approach for constructing detector response functions, which consisted of a number of separable features that include:

- full energy Gaussian peak,
- a single Gaussian escape peak,
- a double Gaussian escape peak due to annihilation photons,
- one or two exponential tails on the low-energy side of the full energy peak,
- a flat continuum that ranges from zero to the full energy peak,
- a Compton scattering continuum from zero to the full energy peak,
- a Compton scattering continuum between the first and second escape peaks, and
- X-ray escape peaks from detector component element such as Ge, Si, and I.

The semi-empirical method was applied successfully for Ge and low-energy Si (Li) detectors (He et al., 1990), but it is limited in practical use because it is a specified approach for some detectors but not all detectors are suitable to use this method, especially when high energy γ-rays are involved.

* Corresponding author. Tel.: +1 832 626 7909.
E-mail address: fusheng.li@bakerhughes.com (F. Li).

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In the 1970s, Berger and Seltzer (1972) started to use Monte Carlo simulations to calculate and develop the response function of NaI(Tl) detectors. In the recent years, the MCNP [Version 5, 2003] program and other Monte Carlo programs such as GEANT4 are used to generate detector response functions for commonly used γ-ray scintillation detectors and are suitable for various source form factors and arbitrary geometry setup. However, the detector response functions generated from these general-purpose Monte Carlo simulation codes are not accurate enough for some spectrometry applications. Therefore, the author of this paper developed a specific-purpose γ-ray detector response function (GAMDRF) code to calculate accurate detector response functions that considers and implements the following nuclear interaction features into the code:

- Photoelectric absorption (PE).
- Compton scattering (CS).
- Rayleigh scattering.
- Pair production (PP).
- X-ray fluorescence and Auger electron.
- Bremsstrahlung radiation by electrons.
- Doppler effects on Compton scattering.
- Electron production by PE, CS, PP, etc., and a semi-empirical electron transportation model.

Electron transportation modeling in MCNP is a time-consuming process. To speed up the simulation and improve the detector response functions' accuracy, a special electron transport model was implemented in the Monte Carlo simulation code with semi-empirical electron transportation parameters optimized to match experimental spectrum. Once the parameters are determined for a specified detector, this specific-purpose Monte Carlo code can be used to generate a series of detector response functions with improved accuracy for energy up to 10 MeV or higher.

2. Theory

The detector response function (DRF) is defined as the pulse height distribution for incident mono-energetic γ-ray, usually indicated by $R(E', E)$, where E' is the pulse height energy and E is the incident γ-ray energy. Traditionally, the DRFs are a set of probability distribution functions that are always larger than or equal to zero over their entire range and integrate over all E' to unity. GAMDRF is not only able to provide the spectral probability distribution functions, but it also calculates detection efficiency for each pulse height energy, which is very important information for the enhanced pulse height tally modeling that convolves the detector surface flux spectrum with DRFs to generate the pulse height spectrum using the following procedure (Fig. 1):

- The surface flux spectrum on the detector surfaces is generated by MCNP or other Monte Carlo simulation software, where only γ-rays entering the detector are tallied and those exiting the detector surfaces are not recorded.
- Detector response functions are produced by GAMDRF code according to the detector type and detector dimensions and convolved with the surface tally obtained from the first step. The outcome of this step is pulse height spectrum without Gaussian energy broadening.
- Then the pulse height spectrum obtained at previous step is processed by Gaussian Energy Broadening, and the final result is the pulse height spectrum that is comparable to real experimental data.

The convolution of surface flux spectrum $\Phi(e)$ and DRFs is defined as the integral of the product of two functions after one is reversed and shifted. As such, pulse height spectrum is a particular kind of integral transform,

$$PulseHeight = (\Phi * \mathrm{DRF})(E) = \int_{E\min}^{E\max} \Phi(e)\mathrm{DRF}(E-e)de$$

Monte Carlo models are a class of computational algorithms that rely on repeated random sampling to compute their results. The simulation code (GAMDRF) is designed to track each particle's life cycle from its birth to end. Comprehensive nuclear physics models for the γ-ray transportation and interaction are applied to determine each particle's property (energy, weight, direction, position, etc.) on each interaction. The amount of the energy deposited in the detector is recorded and tallied to form the pulse-height tally (i.e., detector response function) for each mono-energetic γ-ray. Generally, millions of such particles are simulated and the mean behavior of these particles' random contributions generates meaningful detector responses. The mono-energetic γ-ray source is defined as point source or surface source surrounding the detector. A source direction biasing technique is used to improve the simulation efficiency. Only those γ-rays entering detector are counted to calculate the detector efficiency accurately. Usually, pulse height spectra using mono-energetic γ-ray sources are also measured in laboratory and the Monte Carlo models are benchmarked with experimental data to guarantee the accuracy of the modeling.

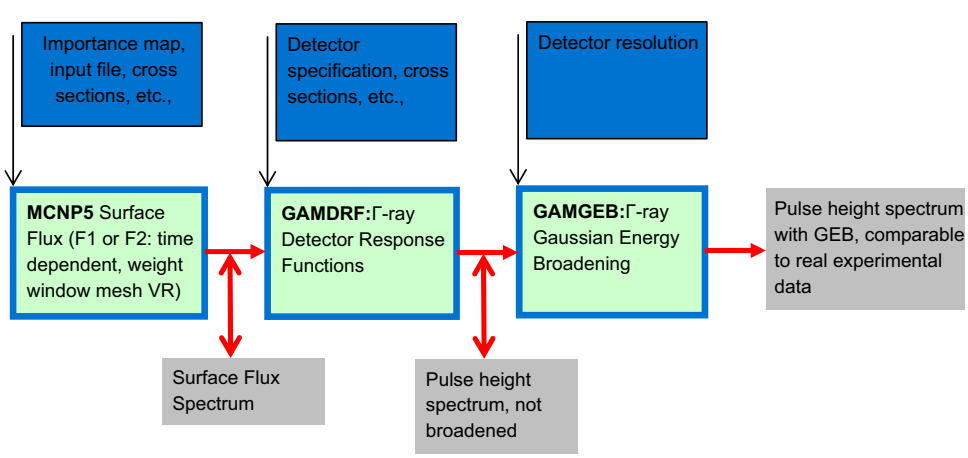

Fig. 1. Enhanced pulse height tally using detector surface spectrum in conjunction with DRFs.

General-purpose Monte Carlo codes like MCNP can be used to calculate detector response functions. However, it is not adequate to generate the DRFs in a fast and accurate manner when electron transportation process in MCNP is turned on. It is very time consuming and makes the generation of accurate DRFs almost impossible in a reasonable time. In addition, the comparison between MCNP calculated DRFs and the experimental spectrum shows there is discrepancy at the flat continuum from zero to photon energy peak. To address the required accuracy and speed of computed DRFs, GAMDRF has been designed to simulate the response of a bare (or enclosed) detector crystal (such as NaI, BGO, $LaBr_3$(Ce), etc.) to a mono-energetic source. The advantage of this code is its capability of generating the response functions of different kinds of detector crystals and detector dimensions in a fast and accurate way. This is because it incorporates all necessary γ-ray interaction nuclear physics mechanisms and a semi-empirical electron transportation treatment with adjustable parameters to match the experimental spectrum for a specific detector crystal or dimension. After the semi-empirical parameters are optimized, GAMDRF can calculate the DRFs very quickly and accurately to match experimental values. Furthermore, the contribution to the pulse height tally from physical mechanisms such as Compton scattering, Rayleigh scattering, single and double of photon escape due to pair production and annihilation, X-ray fluorescence photon escape, etc., can be studied in great detail. This replaces the approximations introduced in semi-empirical models such as neglecting attenuation in the contribution from multiple Compton scattering. This feature enables an accurate DRF to be used in characterizing the detector response, and the differences in experimental and predicted responses can be explained by examining the contribution of each individual component.

3. Method

The Monte Carlo calculation in GAMDRF includes basic γ-ray interactions and electron transportation features: photoelectric absorption (PE), Compton scattering (CS), pair production (PP), X-ray fluorescence and Auger electron generation and escape, Bremsstrahlung radiation, Doppler effects on Compton scattering, electrons production by PE, CS, PP, etc., and semi-empirical electron transportation. Nuclear cross sections are obtained from the Evaluated Photon Data Library (EPDL97), and atomic relaxation data for electrons and photons are from Evaluated Atomic Data Library (EADL), which are based on the ENDF-6 format.

The Monte Carlo models for photoelectric absorption, Compton scattering, pair production, X-ray fluorescence, etc., are similar to those general-purpose Monte Carlo modeling codes such as MCNP. The electron transport model treatment is different and begins with a calculation of the range of the electron, following the form:

$$R = \frac{aE^{b-c\ln(E)}}{\rho}$$

where R is in cm, E is in MeV, and ρ is in g/cm^3. The parameters a, b, and c are empirically determined values by matching the computer-predicted spectrum with the experimental spectrum.

The electron collision was approximated by assuming the path begins as a straight line with continuous energy loss by ionization until a major interaction occurs and changes the original direction. The electron loses energy continuously by ionization collisions moving along this distance. The new energy of the electron due to the ionization collisions can be calculated using the range relationship above and solving for the new energy E'. The energy deposited in the detector is the difference between the original electron E and E'. Changing the direction of the electron contributes to the radiative energy loss of the electron by the production of Bremsstrahlung radiation, which is modeled by a thick target model. Radiative energy loss is dominant for electrons at higher energies, while collisional energy loss is dominant for lower energies and is characterized by the stopping power.

The energy resolution for a scintillation detector is defined as

$$R = \frac{\mathrm{FWHM}}{E_0}$$

where FWHM is full width at half maximum of the photopeak and E_0 is the photopeak energy. The statistical distribution for photopeak is approximated by normal function:

$$g(E) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(E-E_0)^2}{2\sigma^2}\right]$$

where σ is the standard deviation of the photopeak and E_0 is the photopeak energy. The relationship between FWHM and the standard deviation is

$$FWHM = 2.35482\sigma$$

For the detector photopeak standard deviation (σ), a proper regression function to experimental is given as

$$\sigma = aE^b + c$$

The parameters a, b, and c are empirically determined by matching experimental spectral standard deviation (σ) at each photopeak energy (E). Fig. 2 shows the detector standard deviation (σ) variation with energy (E) for three detector crystals: $LaBr_3$(Ce), NaI, and BGO.

After the detector's spectral resolution is determined and its DRFs are calculated, spectrum convolution is used to convert the Monte Carlo computed γ-ray surface flux energy spectrum to the pulse height spectrum with the help of DRFs. Gaussian broadening code is then applied on the pulse height spectrum to make it comparable to the experimental spectrum. Matlab-based GUI codes are developed for spectrum convolution and Gaussian broadening. Fig. 3 shows the GUI interface of Matlab codes for such purposes. For Gaussian broadening, users must input two or more pairs of peak standard deviation (σ) with associated photopeak energy. This code can also deal with the non-linearity of the γ-ray energy spectrum. Fig. 4 demonstrates the detector response functions for cylindrical NaI with its diameter 1.5 in. and a height of 4 in. As incident γ-ray energy increases, the overall detector efficiency decreases, and double and single photon escape peaks are more obviously observed due to annihilation photons.

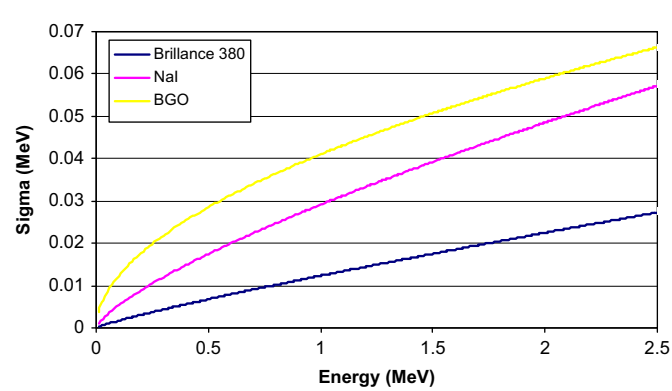

Fig. 2. Detector standard deviation (σ) relationships with energy for three detectors (LaBr3, NaI, and BGO).

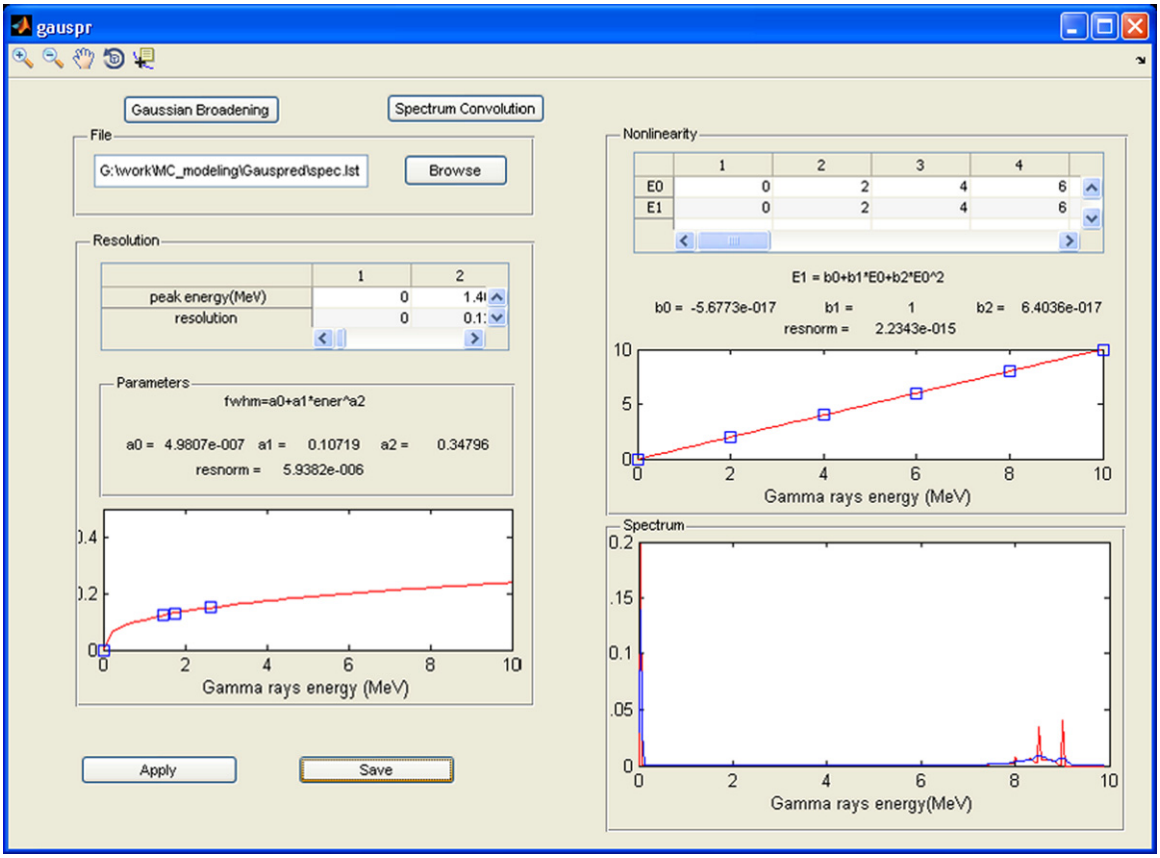

Fig. 3. Matlab GUI code for spectrum convolution and Gaussian energy broadening.

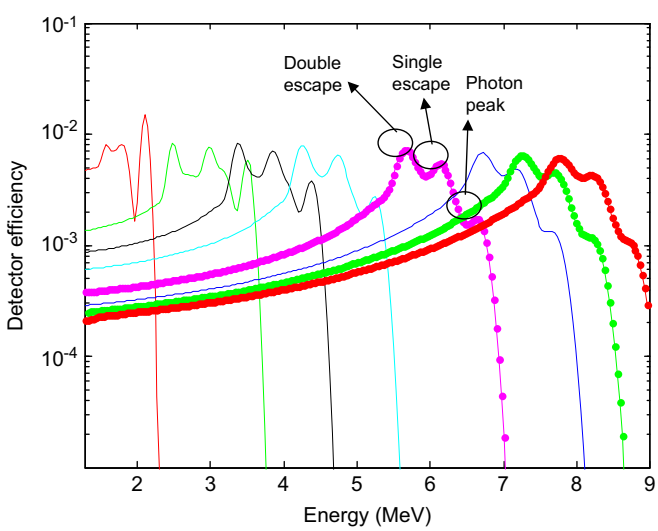

Fig. 4. Detector response functions for NaI detector with dimension 1.5 in. × 4 in.

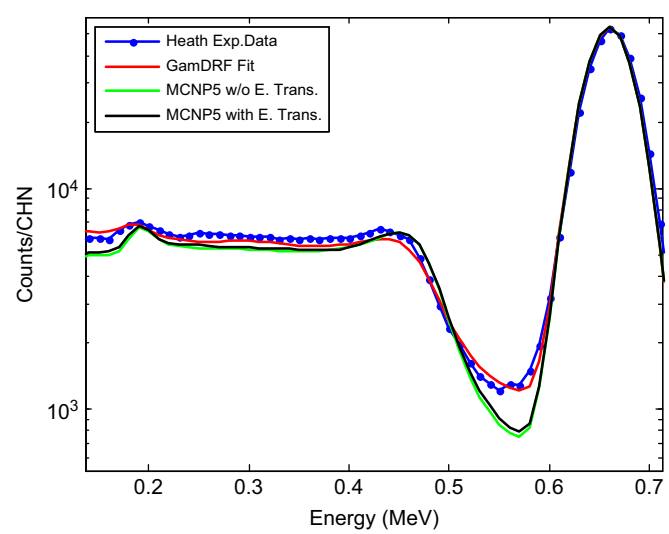

Fig. 5. Calculated NaI DRFs by GAMDRF and MCNP compared with experimental spectrum for ^{137}Cs (E=0.661 MeV).

4. Results and analysis

The calculated DRFs with GAMDRF and MCNP5 were compared with experimentally measured spectra to prove the accuracy of the computed DRFs. The DRFs to γ-ray radioisotopes of ^{137}Cs (E=0.661 MeV), ^{54}Mn (E=0.834 MeV), ^{22}Na (E=1.273 MeV), ^{41}Ar (E=1.293 MeV), ^{60}Co (E_1=1.173 MeV, E_2=1.332 MeV), ^{28}Al (E=1.778 MeV), and ^{37}S (E=3.13 MeV) have been obtained using the Monte Carlo methods (GAMDRF and MCNP5) and compared to DRFs of the experimental values for NaI detector (Heath, 1964) or BGO detector from laboratory measurements. As seen in Figs. 5 and 6, the experimental and calculated DRFs by GAMDRF are in very good agreement. However, the DRFs calculated by MCNP5 are different from experimental DRFs, especially in the flat continuum region of the spectra. For MCNP5-calculated DRFs, both options with electron transportation and without are shown. As observed, MCNP5-calculated DRFs, even with electron transportation option turned on, are not sufficient when compared with experimental spectrum. Although MCNP calculated DRF (e.g. ^{37}S) with electron transportation is better than those without electron transportation, they are still worse than GAMDRF-calculated values in the flat

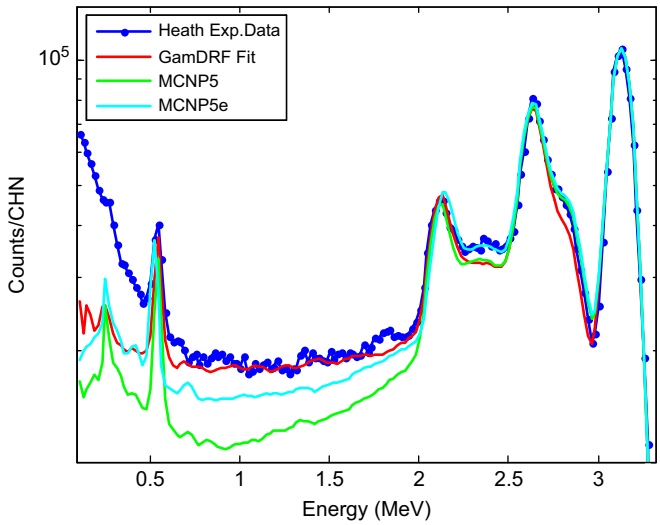

Fig. 6. Calculated NaI DRFs by GAMDRF and MCNP compared with experimental spectrum for ^{37}S (E=3.13 MeV).

continuum region, and MCNP computation with electron transportation is very slow and impossible to use in real practice when time is critical. Therefore, the GAMDRF has better performance in calculating accurate DRFs as this code incorporates all required γ-ray interaction nuclear physics and semi-empirical electron transpiration with adjustable parameters to match experimental data. More results are shown in Figs. 7 and 8 for ^{41}Ar and ^{28}Al, respectively, and they are in good agreement.

Experiments were also performed on BGO detector (3 in. × 3 in.) to benchmark GAMDRF code with four chemical radioisotopes: ^{137}Cs, ^{54}Mn, ^{22}Na, and ^{60}Co. The sources were positioned at 5 cm away from the axis of cylindrical detector and a measurement of the spectrum with 10 min was taken to obtain the energy spectrum for each isotope. The results were compared with the computed DRFs from GAMDRF. The results are shown in Figs. 9 and 10 for ^{137}Cs and ^{22}Na, respectively. It is observed that the computed spectrum by GAMDRF and the experimental spectrum agree with each other very well. In the case of ^{60}Co, the source emits two different γ-rays with the energies of E_1=1.173 MeV and E_2=1.332 MeV. GAMDRF is used

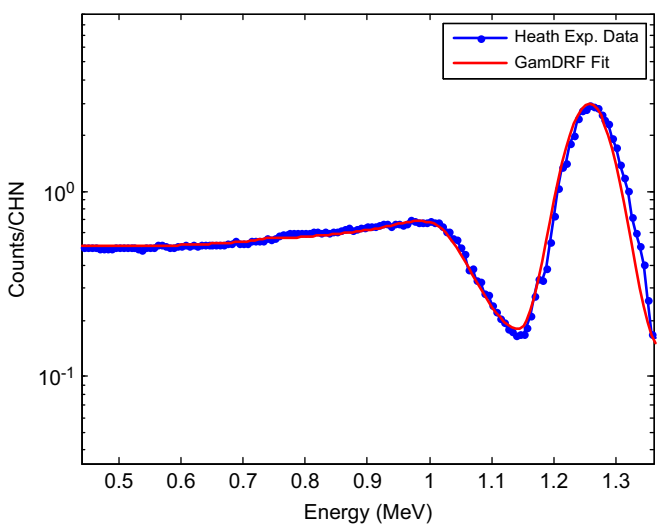

Fig. 7. Calculated NaI DRFs by GAMDRF compared with experimental spectrum for ^{41}Ar (E=1.293 MeV).

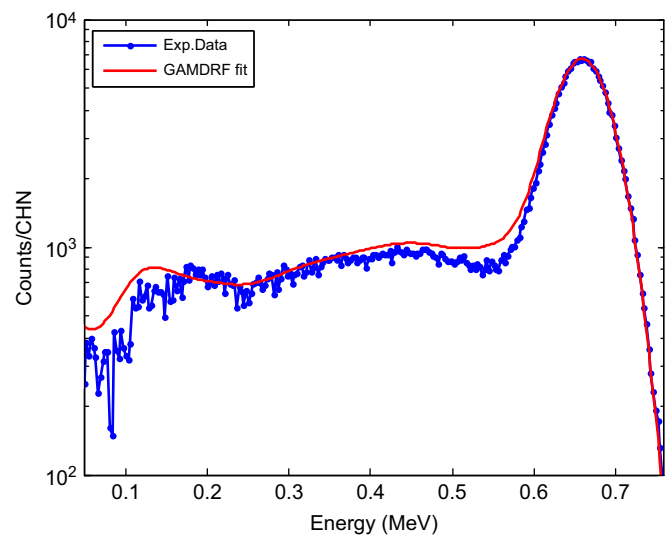

Fig. 9. Calculated BGO DRF by GAMDRF compared with experimental spectrum for ^{137}Cs (E=0.661 MeV).

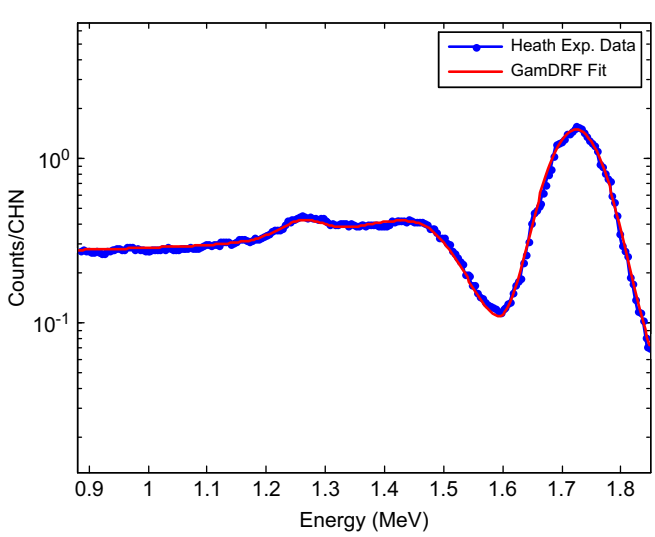

Fig. 8. Calculated NaI DRFs by GAMDRF compared with experimental spectrum for ^{28}Al (E=1.778 MeV).

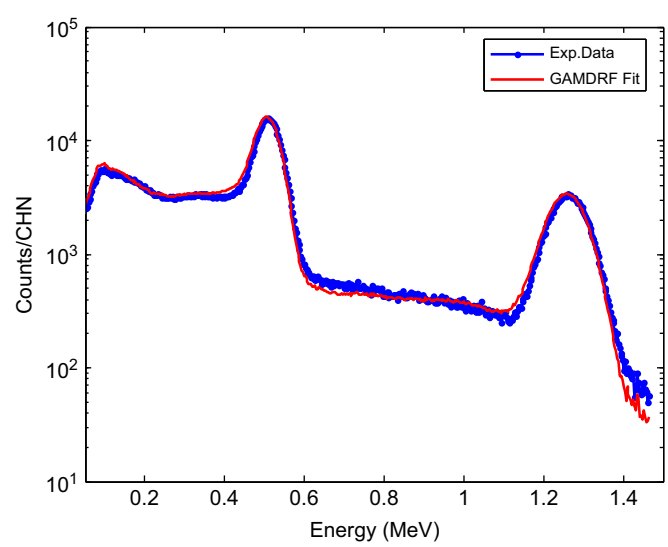

Fig. 10. Calculated BGO DRF by GAMDRF compared with experimental spectrum for ^{22}Na (E=1.273 MeV).

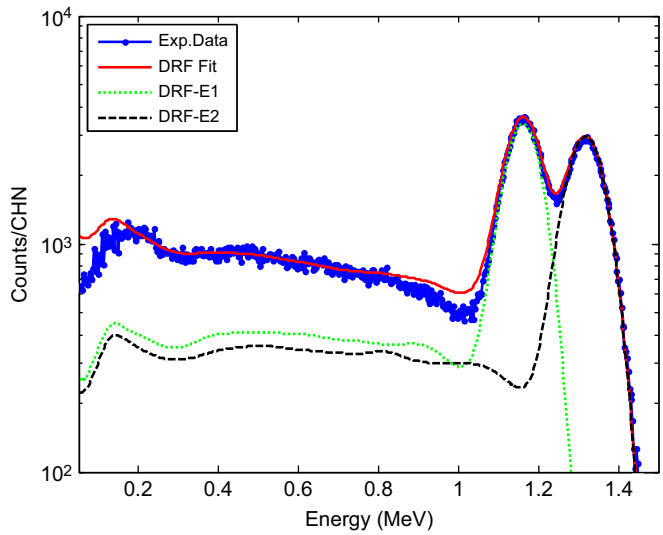

Fig. 11. Calculated BGO DRF by GAMDRF compared with experimental spectrum for ^{60}Co (E_1=1.173 MeV and E_2=1.332 MeV).

to generate two DRFs corresponding to E_1 and E_2. Then they are processed by Gaussian energy broadening and used to regress with the experimental spectrum (with background subtracted). The results are shown in Fig. 11, which demonstrates GAMDRF-computed DRFs fit the experimental spectrum very well.

5. Conclusions

A Monte Carlo-based γ-ray detector response functions code (GAMDRF) was proposed and implemented for NaI, BGO, $LaBr_3$(Ce), etc., detectors with arbitrary dimensions and variable source positions. The code incorporates complete photon interaction mechanisms and a special semi-empirical electron transportation simulation to match the experimental detector response function with adjustable parameters.

The γ-ray spectra produced by several chemical radioisotope sources were measured in the laboratory using three detectors (NaI, BGO, and $LaBr_3$(Ce)). The GAMDRF code is used to produce detector spectral responses according to the experiment setup. The simulated detector response spectra were processed by Gaussian energy broadening code (GAMGEB) and compared with experimental spectra. For comparison purposes, MCNP was also used to produce the spectral response based on the same setup. The comparison results demonstrated that GAMDRF matched the experimental spectra very well. The method is useful to provide enhanced pulsed height tally and the spectral de-convolution process, which is especially important for development of nuclear spectrometry tools in oilwell logging.

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