Technical note

Aspects of GEANT4 Monte-Carlo calculations of the BC501A neutron detector

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Abstract

The response function of a commercial 2 in. $\times$ 2 in. BC501A neutron detector has been studied through the general-purpose Monte-Carlo (MC) simulation toolkit GEANT4. For neutron energies below 8 MeV, where the dominant detection mechanism originates from the knockout protons, the results of MC calculations reproduce remarkably well the experimental pulse-height spectra. This is not the case, however, at higher neutron energies, where the contribution of heavier charged particles to the detection mechanism becomes significant. The calculated detector efficiency is also compared at three indicative energies to the experimental one via the neutron activation technique.

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1. Introduction

One of the most widely used neutron detectors in the fast neutron energy region is the organic liquid scintillator BC501A (or NE213). The BC501A neutron detector is used for neutron monitoring, time-of-flight (TOF) measurements and neutron spectroscopy measurements, mainly due to its excellent n - γ discrimination properties, fast time response and high detection efficiency. This detector has been extensively studied in literature, e.g., Refs. [1,2].

Pioneer sophisticated software packages, such as O5S [1], SCINFUL [3] and NRESP [4, and references therein], have been developed in the past, especially designed and adjusted for NE213. These codes take into consideration the full complexity of the light production inside the detector, namely the influence of multiple neutron interactions, wall effects and non-linear light responses for secondary charged particles. Nevertheless, the relative lack of reliable, experimental and/or evaluated differential

cross-sections of neutron-induced reactions in carbon still presents serious challenges, especially for neutron energies above 8 MeV. Moreover, in the case of complicated experimental setups, e.g., heavily shielded detectors exposed to mixed n/γ /muon fields, the applicability of such simulation codes is severely limited [4].

Thus, following the thorough contributions that have been presented recently, implementing MCNP and FLUKA [5,6], the present work aims at studying the applicability of a widely used, general-purpose Monte-Carlo (MC) simulation toolkit, such as GEANT4 [7], for the calculation of the response function of a cylindrical (5.08 cm in height and 5.08 cm in diameter) BC501A neutron detector. Extensive GEANT4 calculations were performed in the incident neutron energy range between ~ 0.5 and 19 MeV and the generated spectra were compared to the experimental pulse-height ones, obtained at $E_n = 5.5, 7.5, 17.4, 17.7$ and 18 MeV. Moreover, the absolute detection efficiency was studied at three indicative incident neutron energies, namely at 5.5, 7.5 and 18.1 MeV. For this purpose, the neutron flux was measured at the detector position with the neutron activation technique.

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2. Experimental setup

2.1. The neutron beam and accelerator facility

The neutron beam was produced via the $^2\text{H}(\text{d}, \text{n})\ ^3\text{He}$ reaction, by bombarding the ^2H gas target [8] with the deuteron beam delivered by the 5.5 MV Tandem Van de Graaff accelerator of the National Center for Scientific Research “Demokritos”. A 5- μm molybdenum foil served as the entrance window and a Pt foil as the beam stopper of the gas cell. During the irradiations, the gas target was cooled through a cold air jet, in order to minimize the effect of heating in the deuterium gas pressure, which was continuously controlled through a micrometric valve. By varying the deuteron beam current, the neutron flux was adjusted as to keep the counting rate at the BC501A neutron detector at tolerable levels.

Higher neutron beam energies were achieved via the $^3\text{H}(\text{d}, \text{n})\ ^4\text{He}$ reaction. In this case, a solid tritiated-titanium target was used. During the irradiations, the solid target was rotated to avoid the continuous bombarding of the same target point, which could cause target deterioration. The target was also cooled by using lateral heat conduction from the Al beam dump to the surrounding pressured cold air channel.

In all cases, the separation of neutron-induced events from γ -ray events was achieved using conventional pulse-shape discrimination (PSD) electronics.

2.2. The neutron activation measurements

For the experimental determination of the neutron detection efficiency of the 2 in. $\times$ 2 in. BC501A detector, the absolute neutron flux was measured via the neutron activation technique. The efficiency of the detector was experimentally deduced for three neutron beam energies: At 5.5 and 7.5 MeV (using the $^2\text{H}(\text{d}, \text{n})\ ^3\text{He}$ reaction), and at 18.1 MeV (through the $^3\text{H}(\text{d}, \text{n})\ ^4\text{He}$ reaction). In all cases, the effect of low-energy scattered neutrons from the floor and surrounding materials was relatively minimized by a detector shield made of heavy paraffin and cadmium (paraffin cylinder $\sim$ 1 m long, with an outer/inner diameter of $\sim$ 60/7 cm, fully covered by Cd foils), in conjunction with the small solid angle subtended by the detector (placed at the far end of the shielding). Neutrons at intermediate energies (between 7.5 and 18.1 MeV) could only be produced via the $^2\text{H}(\text{d}, \text{n})\ ^3\text{He}$ reaction by increasing the bombarding deuteron energy. However, for higher deuteron energies, the contribution of parasitic low-energy neutrons originating from deuteron break-up and/or from deuteron induced reactions with the structural materials of the gas target becomes significant. These effects increase strongly the inaccuracy of the comparison with the simulated data [9], in the absence of additional TOF capabilities.

During the irradiations, the BC501A neutron detector was exposed to the neutron field together with a reference

activation foil. The choice of the reference foil depended on the incident neutron energy and on the following constraints: (a) well-known reaction cross-section, (b) high reaction rate, and (c) smooth excitation function. Thus, for the 5.5, 7.5 and 18.1 MeV irradiations, the reference reactions were $^{115}\text{In}(\text{n}, \text{n}')\ ^{115\text{m}}\text{In}$ [10], $^{27}\text{Al}(\text{n}, \alpha)\ ^{24}\text{Na}$ [11], and $^{90}\text{Zr}(\text{n}, 2\text{n})\ ^{89}\text{Zr}$ [11], respectively.

The induced activity of the samples was measured by a 56% relative efficiency HPGe detector. The absolute efficiency calibration of the HPGe detector was measured with a calibrated ^{152}Eu point source (at 2.4% accuracy), set at the same position as the activated foil. The source to detector distance was 9–10 cm (depending on the measurement). At this distance, any corrections for pile up and coincidence-summing effects were well below all other sources of uncertainty.

The neutron flux at the entrance window of the BC501A neutron detector was calculated by normalizing the solid angle subtended by the reference foil with respect to the corresponding one subtended by the neutron detector.

3. GEANT4 Monte-Carlo simulations

The response function of the BC501A neutron detector was calculated by means of the GEANT4 detector simulation toolkit [7]. For these MC calculations, the full geometry of the detector container and the chemical composition of the liquid scintillator were taken into account. The photomultiplier tube was ignored, since only the energy deposit of the recoiling particles was scored. GEANT4 simulates neutron transport from thermal energies up to 20 MeV. Neutron capture, fission, elastic and inelastic scattering (including absorption) are treated by referring to the ENDF-B VI cross-section data. Recent comparisons with MCNP [12], demonstrate the validity of GEANT4 calculations in neutron generation and transport. Moreover, object-oriented programming and highly sophisticated processing of both electromagnetic interactions and ionization processes enhance GEANT4 capabilities for the study of mixed fields and complicated geometries.

It should be noted that, for the BC501A detector, a light output function has to be folded with the simulated results in order to compare them with the experimental pulse-height spectra. This function differs significantly for the secondary particles (p, α , ^{12}C , ^9Be , etc.) generated in the detector by the impinging neutrons. One more complication arises from the fact, that the light output function for each particle is not linear, especially for low incident neutron energies. For neutron energies lower than $\sim$ 8 MeV, the main detection mechanism can be attributed to recoil-protons, since the light yield of heavier emitted or recoil particles is much smaller, and in most cases well below the ADC threshold. However, this assumption does not hold anymore above $\sim$ 8 MeV. The problem is even more complicated, if one takes into account the uncertainties of the evaluated differential cross-sections of

the $n + {}^{12}\text{C}$ reactions. In the present work, as a first-order approximation, only the recoil protons were taken into account over the whole energy range, and thus, only a single light output function was considered. Therefore, the proton energy (E_p) deposit inside the scintillator material was scored and transformed to light output (in channels—arb. units) according to Eq. (1) (e.g., Ref. [13]):

$$L(\text{Chan.}) = AE_p + BE_p^2, \quad (1)$$

where the coefficients A , B were estimated through the direct comparison of the experimental pulse-height spectra with the calculated ones. More specifically, the linear part of the above function was determined from the higher end of the experimental pulse-height spectra, where the mid-point of the slope of the high-energy end of the spectra corresponds to the neutron beam energy. Multiple scattering on carbon (with an energy loss of the scattered neutron up to 24% and negligible light production by the recoil carbon) and subsequently on hydrogen, strongly influences the shape below the upper edge, in particular for neutron energies below 8 MeV (see Figs. 8a and b in Ref. [4]). In case of multiple scattering on hydrogen, the non-linear light output for protons also influences the shape of the spectrum, because the light output is calculated for each recoil-proton individually and then summed up to the total light output for one neutron history. The non-linear part of the function mainly affects the lower part of the calculated spectrum and was adjusted to achieve the best possible agreement between the experimental and the calculated pulse-height spectra.

At higher neutron energies (> 17 MeV), the contribution of the ${}^{12}\text{C}(n, p){}^{12}\text{B}$ reaction channel becomes evident. This second group of protons was used as an extra calibration point for estimating the light output function of the recoil protons. It should be noted that in GEANT4 MC calculations, the evolution of protons originating from this reaction was accurately followed. In this energy region, a different set of A and B parameters (Eq. (1)) was calculated, since some parameters of the electronic chain had to be changed.

The detector resolution was also taken into account as a function of light emission, i.e., pulse height. A random quantity was added to the calculated light pulse height, extracted from a zero-centered Gaussian distribution with standard deviation equal to the corresponding pulse-height resolution ΔL . The detector resolution function ($\Delta L \propto \sqrt{L}$) was estimated from the experimental spectra, and more specifically from the slope of the higher edge of the pulse-height spectrum.

4. Results and discussion

The results of GEANT4 MC calculations are shown in Fig. 1 for 5.5 and 7.5 MeV neutrons, along with the corresponding experimental pulse-height spectra, normalized according to the sum of the experimentally recorded

Fig. 1. Experimental and GEANT4 MC simulated pulse-height spectra for incident neutron energies below 8 MeV, namely at 5.5 and 7.5 MeV. The calculated spectra were normalized to the experimental ones. The ADC thresholds are indicated by arrows.

events. For these neutron energies, the calculated pulse-height spectrum reproduces the experimental one remarkably well, although only recoil protons were taken into account. This behavior was not surprising since at these neutron energies any pulse attributed to recoil ${}^{12}\text{C}$ or α -particles is expected to be below the ADC threshold. This implies that a general purpose code such as GEANT4, can be used to simulate the detector response function in this energy region, simply by converting each proton energy deposition into light and, in case of multiple n-p scattering, adding up the light for one neutron history.

The same procedure was followed at higher neutron energies (17.4, 17.7 and 18.0 MeV). The experimental pulse-height spectra (for the same accumulated beam charge on target) are shown in Fig. 2 together with the simulated ones. At this neutron beam energy region, the MC calculations reproduce fairly well only the higher part of the pulse-height spectrum which is attributed to recoil protons. The contribution of heavier particles (α , ${}^{12}\text{C}$, d, ${}^{12}\text{B}$ and ${}^9\text{Be}$) at these neutron energies is significant and

Fig. 2. Experimental and GEANT4 MC calculated pulse-height spectra for incident neutron energies above 8 MeV, namely at 17.4, 17.7 and 18.0 MeV. The calculated spectra were normalized to the experimental ones. The edge appearing in the simulated spectra around channels 300–500 corresponds to recoil protons originating from the $^{12}\text{C}(\text{n}, \text{p})^{12}\text{B}$ reaction. The ADC thresholds are indicated by arrows.

generates lower height pulses. Since in these calculations only the recoil protons have been taken into account, the disagreement between the experimental spectra and the

MC calculations in the lower part of the pulse-height spectra was expected. It should be underlined (Fig. 2) that the discrepancy between the lower part of the spectra increases with neutron energy. Therefore at these energies, the response functions of the BC501A scintillator can be predicted accurately by the simulations, only if all the detection mechanisms are accounted for. Nevertheless, the phenomenological approach adopted in the present work yielded results comparable to those calculated with FLUKA [6]. It should be underlined that also in that work only recoil protons were accounted for. The agreement with the experimental data was satisfactory over a broad energy range (5.5–18 MeV). Another work [5] adopted an extended version of MCNP which includes additional reactions, such as $^{12}\text{C}(\text{n}, \text{n}'^3\alpha)$. The angular distribution of the emitted α -particles was assumed to be isotropic. A specific light output function was used for each secondary particle. The agreement with the experimental spectra generated by 14 MeV neutrons was excellent. It is doubtful, however, whether such assumptions hold over a wide energy range. It is the authors' firm belief that further work is required for the accurate calculation of the response functions, by accounting for all the contributing reactions.

In Table 1, a comparison between the experimental and the simulated absolute efficiency values is presented. As already mentioned, the neutron flux was measured with the neutron activation technique. The efficiency of the BC501A scintillator (for various detector sizes and ADC thresholds) has also been determined in many works (e.g., Refs. [14–17]), by using the associated particle technique or through well-known differential cross-sections of the neutron producing reactions.

The efficiency data were measured by using n/γ discrimination, with an ADC threshold set as low as possible (at $\sim \frac{1}{4}$ of the ^{137}Cs Compton edge). The detector efficiency values at 5.5 and 7.5 MeV (with a total experimental uncertainty of $\sim 14\%$ and 13% , respectively) are quite close (within 12.5% and 8% , respectively) to those predicted by GEANT4 ($\sim 10^5$ – 10^6 recoil-proton events scored for each neutron energy point, yielding statistical uncertainties of less than 1% in both cases). It has to be noted here that the observed discrepancies are attributed only to the limitations of the activation technique, along with the solid angle normalization, that greatly enhance the total experimental uncertainty in the determination of the absolute efficiency of the detector (as presented in Table 1) and not to the GEANT4 calculations. The simulated results were obtained with the same threshold as the experimental ones and by considering only recoil protons, as mentioned above. However, the high-energy point at 18.1 MeV (total experimental uncertainty $\sim 21\%$) is well above (50%) the GEANT4 calculated efficiency value. This is in agreement with the results shown in Fig. 2, where the contribution of heavier particles to the overall detection efficiency is significant.

Table 1

The experimental efficiency data (points) at $E_{n,\text{lab}} = 5.5, 7.5$ and 18.1 (along with the total combined errors of 14%, 13% and 21%, respectively) are compared to the results of GEANT4 MC calculations (the statistical uncertainties of less than 1% are omitted from the table)

E_n (MeV)	Activated foil	Neutron fluence (n/cm^2)	Absolute efficiency (experimental)	Absolute efficiency (GEANT4)	Ratio
5.5	^{115}In	$(2.50 \pm 0.16) \times 10^{10}$	0.36 ± 0.05	0.32	1.125
7.5	^{27}Al	$(1.50 \pm 0.09) \times 10^{10}$	0.23 ± 0.03	0.25	0.92
18.1	^{90}Zr	$(7.22 \pm 0.26) \times 10^9$	0.24 ± 0.05	0.16	1.5

In these simulations only the contribution of the recoil protons has been taken into account.

5. Conclusions

The experimental pulse-height spectra were compared to the results of GEANT4 MC calculations. Only recoil protons were taken into account in the GEANT4 simulations. The energy deposition of the recoil protons scored in the MC calculations was transformed into light output in arbitrary units, according to the experimental pulse-height spectra. Also, the detector finite resolution as deduced from the experimental spectra was included in the calculations.

It has been shown that for neutron energies below ~ 8 MeV where the dominant detection mechanism is the neutron–proton elastic scattering, GEANT4 MC calculations reproduce the experimental response function quite well. This is a clear indication that GEANT4 MC calculations can be implemented in this energy region in order to reproduce the detector response matrix. Therein-after, the deduced response matrix can be used in a standard deconvolution algorithm in order to obtain the actual neutron beam energy distribution.

At higher incident neutron energies, however, the lower energy part of the simulated pulse-height spectra is underestimated, since the contribution of the heavier particles to the overall detection mechanism is expected to be critical. Thus, further work is required in both theoretical and experimental fields in order to account for the observed discrepancies.

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