A FAST, PRIMARY-INTERACTION MONTE CARLO METHODOLOGY FOR DETERMINATION OF TOTAL EFFICIENCY OF CYLINDRICAL SCINTILLATION GAMMA-RAY DETECTORS

by

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A primary-interaction based Monte Carlo algorithm has been developed for determination of the total efficiency of cylindrical scintillation γ-ray detectors. This methodology has been implemented in a Matlab based computer program BPIMC. For point isotropic sources at axial locations with respect to the detector axis, excellent agreement has been found between the predictions of the BPIMC code with the corresponding results obtained by using hybrid Monte Carlo as well as by experimental measurements over a wide range of γ-ray energy values. For off-axis located point sources, the comparison of the BPIMC predictions with the corresponding results obtained by direct calculations as well as by conventional Monte Carlo schemes shows good agreement validating the proposed algorithm.

Using the BPIMC program, the energy dependent detector efficiency has been found to approach an asymptotic profile by increasing either thickness or diameter of scintillator while keeping the other fixed. The variation of energy dependent total efficiency of a 3"   3" NaI(Tl) scintillator with axial distance has been studied using the BPIMC code. About two orders of magnitude change in detector efficiency has been observed for zero to 50 cm variation in the axial distance. For small values of axial separation, a similar large variation has also been observed in total efficiency for ^{137}Cs as well as for ^{60}Co sources by increasing the axial-offset from zero to 50 cm.

Key words: scintillation detector, total efficiency, point source, Monte Carlo simulation

INTRODUCTION

Precise values of detector total efficiency are required for a variety of applications ranging from environmental radioactivity measurements, trace element quantification by neutron activation analysis, reactor coolant activation studies to cosmic radiation analysis. Normally, along with other parameters, the values of total efficiency are also required for quantification purposes [1].

As standard practice, values of detector efficiency are measured using various calibration sources. This technique works well for mono-energetic gamma-ray sources. However, it is difficult to span any arbitrary desired energy range with such sources adequately. Therefore, typically, suitable interpolation procedure is required for estimation of total efficiency at the desired values of energy [2]. In the absence of a theoretical or well-founded empirical formula, the limited number of calibration points, along with the corresponding experimental uncertainties, tends to make interpolation strategies prone to oscillation tendencies and sensitive to experimental and calibration errors [3].

In the past, efforts have been made for theoretical determination of the values of total efficiency for a variety of situations. These efforts can be divided into three broad categories: analytical methods, stochastic simulation methods, and hybrid techniques. In the case of analytical methods, there are two sub-categories: semi-empirical techniques and direct methods. The work done by [3-14] belongs to the semi-empiri-

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cal techniques. Typically, in these techniques, a "characteristic", and a "correcting" pair of curves are used. The parameters of both curves are determined from experimental measurements by the least-square method. The characteristic curve generally has a relatively small number of parameters requiring only a few points for calibration. The correction curve is constructed using the residuals. Due to its robustness and precision with selectable accuracy, it is recommended by both [15, 16]. Clearly, the semi-empirical techniques are limited by the accuracy of the experimental measurements and the calibration energy range.

In the case of the direct method for determination of total efficiency of detectors, estimates of solid-angle in the source-detector geometry are essential. This involves rigorous mathematical treatment of photon absorption in various directions and often leads to quite lengthy mathematical expressions. The work done by various researchers [17-24] belongs to the class of direct methods for total efficiency determination. These methods represent standard techniques against which all other methods should be benchmarked. However, their extension and applications to situations even slightly deviating from the standard ones pose challenge of carrying-out length mathematical manipulations.

In contrast with the direct methods, the stochastic methods offer easy extendibility for handling very complex geometries [25, 26]. Many researchers have contributed to determination of total efficiency of gamma-ray detectors using Monte Carlo methods. The efforts of [1] and of [27-30] show the effectiveness of Monte Carlo methods in this area.

A lot of work has been done to develop general purpose Monte Carlo simulation codes and currently, many such sophisticated codes are available. These include EGS [31], MCNP [32], GEANT [33], and PENELOPE [34]. The general purpose codes generally require detailed knowledge of the code itself in order to use it for a specific application. Also, they are sometimes tested only on a specific platform which tends to limit their applicability to practical cases. Recently, Yalcin *et al.* [35] have proposed a hybrid Monte Carlo technique which is based on analytical geometry details in conjunction with Monte Carlo procedure in order to improve computational efficiency. However, the extension of this technique to a variety of practical cases remains difficult since it requires elaborate analytical calculations for new geometries.

In this paper, we present the details of a fast, primary-interaction Monte Carlo algorithm for determination of total efficiency of cylindrical scintillation gamma-ray detectors. The computation cost of Monte Carlo simulations is minimized by employing primary-interaction based scoring technique, which requires photon tracking up-to first interaction point only. Additionally, the biasing of photon histories toward scintillation detector has been used to attain fast convergence rates. The proposed algorithm offers easy extendibility while maintaining fast convergence rates for determination of total efficiency of γ-ray detectors.

SIMULATION PROCEDURE

In this work, a cylindrical scintillation detector is considered along with a point isotropic source as shown in fig. 1. The front face of the detector is at distance D from the origin along the z-axis in the axial direction. The detector has radius R and length L while the source is located at point Q having coordinates (x_s, y_s, z_s). It is clear from fig. 1 that the path of photons, emitted only within the range of angle: ϕ $[\phi_{\min}, \phi_{\max}]$ and θ $[\theta_{\min}, \theta_{\max}]$, needs to be tested for intersection with the detector surface. It may be noted that both axially-located as well as off-axial positioned sources are treated in this approach. In these simulations, scattering of photons from surroundings to the detector has been neglected. Also, attenuation of incident photon in the detector "window" is also ignored since it is expected to have negligible affect of total efficiency for the energy range considered here.

Mathematical framework

In these simulations, photons emitted by the point isotropic source have energy E and carry random direction (θ, ϕ) which is biased towards the detector. The polar angle θ has random cosine-sampling in the range [$\theta_{\min}$, $\theta_{\max}$] with r as random number in [0, 1] range

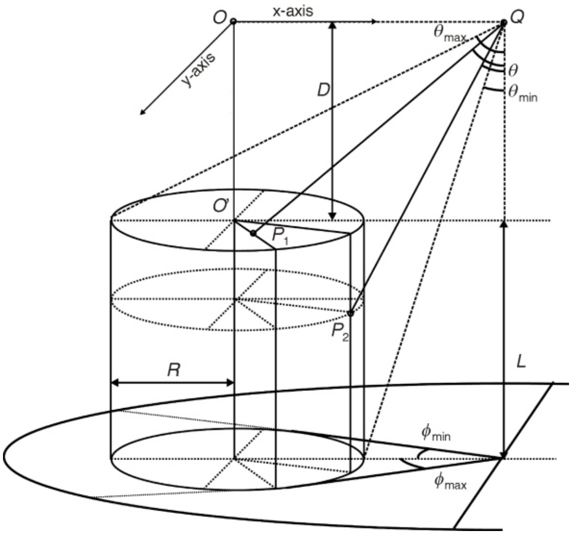

Figure 1. Details of the geometry of a cylindrical scintillator gamma-ray detector and point isotropic source at off-axial location

$$\theta = \cos^{-1}[(1-r)\cos(\theta_{\min}) + r\cos(\theta_{\max})] \qquad (1)$$

where with reference to fig. 1, the range of polar angle θ is found by using

$$\theta_{\min} = \begin{cases} \mathrm{tg}^{-1}[(\rho - R)/(D+L)]; \text{ if } \rho > R \\ 0; \qquad \text{otherwise} \end{cases} \qquad (2)$$

and

$$\theta_{\max} = \mathrm{tg}^{-1}[(\rho + R)/D] \qquad (3)$$

where $\rho = (x_s^2 + y_s^2)^{1/2}$ is the radial distance of the source point from the origin. The azimuthal angle has uniform random sampling from [$\phi_{\min}$, $\phi_{\max}$] range with r as random number in [0, 1] range

$$\phi = (1-r)\phi_{\min} + r\phi_{\max} \qquad (4)$$

where [$\phi_{\min}$, $\phi_{\max}$] are found by using the following set of equations

$$\phi_{\min} = \begin{cases} \mathrm{tg}^{-1}(y_s/x_s) - \sin^{-1}(R/\rho); \text{ if } \rho > R \\ 0; \qquad \text{otherwise} \end{cases} \qquad (5)$$

and

$$\phi_{\max} = \begin{cases} \mathrm{tg}^{-1}(y_s/x_s) + \sin^{-1}(R/\rho); \text{ if } \rho > R \\ 0; \qquad \text{otherwise} \end{cases} \qquad (6)$$

Now, we track the photon and compute its point intersection (x, y, z) with $z = D$ plane which contains the detector upper flat surface. If $(x_s^2 + y_s^2)^{1/2} \le R$, it implies that a photon has entered the detector from the upper flat surface; otherwise, it has passed through the side curved surface (see points P1 and P2 in fig. 1). The coordinates of the point where photon crosses the detector surface are given by (x_d, y_d, z_d). At this stage, the free-flight distance ξ covered by the photon is computed using

$$\xi = -\frac{1}{\mu}\ln r \qquad (7)$$

where μ is the attenuation coefficient of NaI(Tl) detector at energy E and r is random number in (0, 1] range. Then, the coordinates (x_p, y_p, z_p) of the primary interaction point are computed using

$$\begin{aligned} x_p &= x_d + \xi\cos\phi\sin\theta \\ y_p &= y_d + \xi\sin\phi\sin\theta \\ z_p &= z_d + \xi\cos\theta \end{aligned} \qquad (8)$$

The primary interaction point is inside the detector if $(x_p^2 + y_p^2)^{1/2} \le R$ and $D \le z_p \le (D+L)$; and in this case, the photon "score" is incremented by one. This procedure is repeated for N number of photon histories as shown in fig. 2. The total efficiency $\varepsilon_{\mathrm{tot}}(E)$ of the detector is found by using

$$\varepsilon_{\mathrm{tot}}(E) = F_\theta F_\phi \frac{score}{N} \qquad (9)$$

where,

$$F_\theta = \frac{\cos\theta_{\min} - \cos\theta_{\max}}{2} \qquad (10)$$

and

$$F_\phi = \begin{cases} \phi_{\max}/\pi; \text{ if } \rho > R \\ 1; \qquad \text{otherwise} \end{cases} \qquad (11)$$

The values of incoherent total linear attenuation coefficient at various values of γ-ray energies for NaI(Tl) detector were obtained using the XCOM software [36]. A brief list of the values of attenuation coefficient and the corresponding values of mean free paths for these photons obtained from XCOM for NaI(Tl) detector is provided in tab. 1. It is clear from this table that the values of mean free paths are much smaller than the detector dimensions over the gamma ray energy range of interest.

RESULTS AND DISCUSSION

The primary-interaction based Monte Carlo program (BPIMC) with biasing has been used in this work for the calculation of total detection efficiency of cylindrical scintillation detectors with point isotropic γ-ray sources. This program has fast convergence rate and as compared with other standard as well as hybrid Monte Carlo programs which require tracing of 10^6 photon histories, PBIMC program yield converged results typically in 10^4 histories with the standard deviation below 0.4 percent.

The predictions of BPIMC code have been compared with various cases reported in literature. For a 3" × 3" NaI(Tl) detector with point isotropic γ-ray source located at $D = 0.001$, $D = 0.5$, and $D = 10$ cm, the BPIMC computed values of the total detection efficiency have been compared with the corresponding results found by [37-39] and by [17, 35].

The corresponding results show excellent agreement between the prediction of BPIMC code and the corresponding published results as depicted in fig. 3. Numerical values for the three cases at the discrete values of energy are given in tab. 2. Again, it is noted that there is excellent agreement between BPIMC calculated values and the corresponding values found by other indicated researchers.

The primary-interaction based Monte Carlo approach has been used for calculating the energy dependent variation of the total efficiency of 3" × 3" cylindrical NaI(Tl) scintillator for various values of axial distances D and the corresponding results have been shown in fig. 4. Many orders of magnitude change in the total efficiency is observed for variation of D in [0, 50] range. This change may be attributed to change in the solid angle and as well as the change in a number of interactions possible due to oblique to nearly normal incidence of photons.

The BPIMC code has also been used for the calculation of total efficiency values for sources located at off-axial locations at distance ρ from the origin in the perpendicular direction to the detector axis.

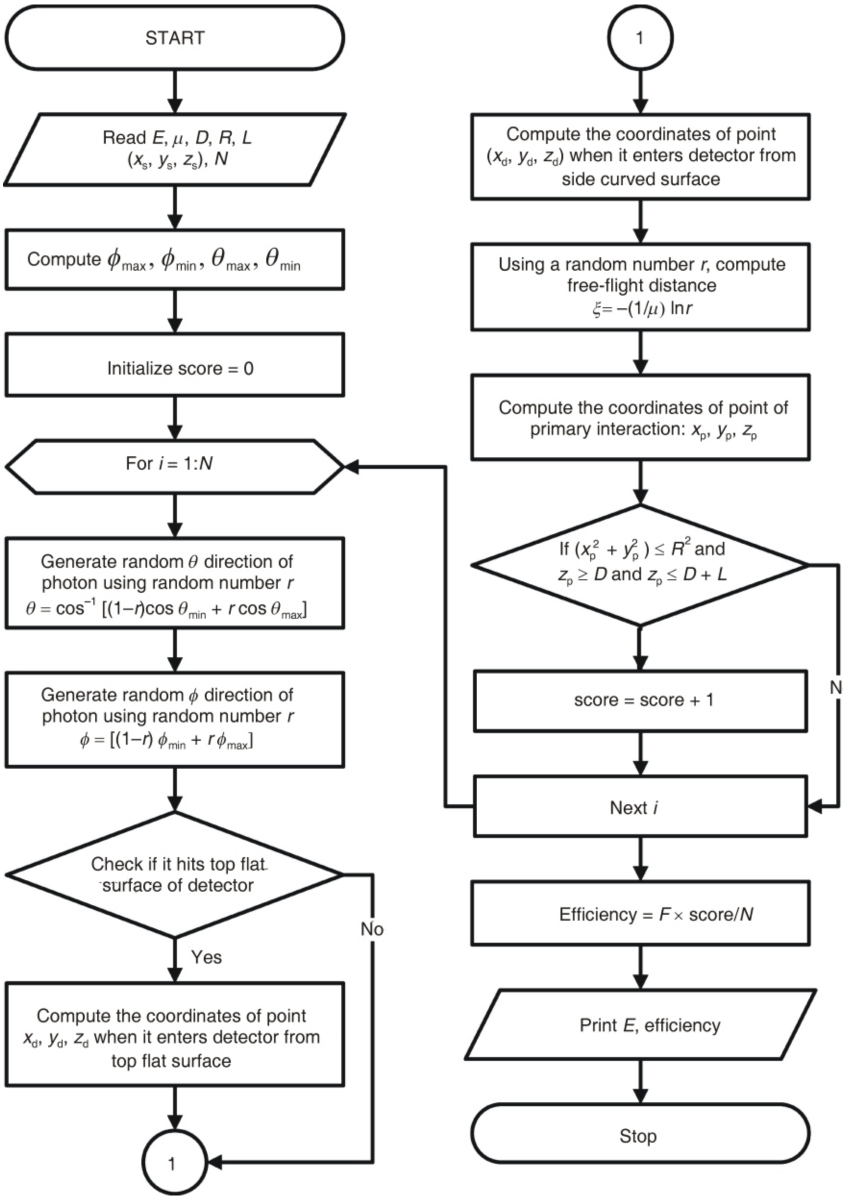

Figure 2. Flow chart of the biased primary-interaction Monte Carlo algorithm

These results have been compared with the calculations of Selim *et al*. [40] and Beam *et al*. [28] for $E\gamma = 0.662$ MeV and are given in tab. 3. It is clear from these data that BPIMC results are in good agreement with the corresponding results found by direct calculations as well as with theoretical and experimental methods.

The variation of total efficiency of the cylindrical scintillation detector for ^{137}Cs and ^{60}Co with axial off-set distance ρ for various indicated values of D is shown in fig. 5. It is observed that the value of total efficiency decreases by increasing the value of ρ as well as D, which is essentially due to reduction in the source-to-detector solid angle. Also, for the same location, the ^{137}Cs source is found to have a higher value of total efficiency as compared with the ^{60}Co source, which is in accordance with the expected behavior, since ^{137}Cs has lower value of photon energy and the corresponding value of total attenuation coefficient (μ) for NaI(Tl) is higher, which leads to a higher value of corresponding total efficiency.

The primary-interaction Monte Carlo based program BPIMC has been used for study of the variation of total efficiency of the cylindrical scintillation detector of various dimensions. In this study, the source has been placed at 5 cm axial location and energy dependent total efficiency values have been calculated for a range of values of the detector thickness and radius. The variation of the energy dependent total efficiency for the 3" dia NaI(Tl) detector with thickness in [1, 10] range are shown in fig. 6. It is observed that total efficiency is independent of detector thickness in the

Table 1. Variation of attenuation coefficient and the corresponding values of mean free path with γ-ray energy [36]

E [keV]	μ/ρ [cm^{2}g^{-1}]	μ [cm^{-1}]	Mean free path [cm]	E [keV]	μ/ρ [cm^{2}g^{-1}]	μ [cm^{-1}]	Mean free path [cm]
1.00E+00	7.76E+03	2.85E+04	3.51E-05	2.00E+02	3.30E-01	1.21E+00	8.27E-01
2.00E+00	1.92E+03	7.04E+03	1.42E-04	3.00E+02	1.67E-01	6.12E-01	1.63E+00
3.00E+00	7.00E+02	2.57E+03	3.90E-04	4.00E+02	1.17E-01	4.29E-01	2.33E+00
4.00E+00	3.36E+02	1.23E+03	8.12E-04	5.00E+02	9.47E-02	3.47E-01	2.88E+00
5.00E+00	7.21E+02	2.64E+03	3.78E-04	6.00E+02	8.20E-02	3.01E-01	3.32E+00
6.00E+00	5.27E+02	1.93E+03	5.17E-04	7.00E+02	7.34E-02	2.69E-01	3.71E+00
7.00E+00	3.56E+02	1.31E+03	7.66E-04	8.00E+02	6.74E-02	2.47E-01	4.05E+00
8.00E+00	2.49E+02	9.13E+02	1.10E-03	9.00E+02	6.25E-02	2.29E-01	4.36E+00
9.00E+00	1.84E+02	6.74E+02	1.48E-03	1.00E+03	5.87E-02	2.15E-01	4.65E+00
1.00E+01	1.40E+02	5.13E+02	1.95E-03	2.00E+03	4.14E-02	1.52E-01	6.59E+00
2.00E+01	2.17E+01	7.94E+01	1.26E-02	3.00E+03	3.67E-02	1.35E-01	7.43E+00
3.00E+01	7.20E+00	2.64E+01	3.79E-02	4.00E+03	3.50E-02	1.28E-01	7.79E+00
4.00E+01	1.87E+01	6.85E+01	1.46E-02	5.00E+03	3.47E-02	1.27E-01	7.87E+00
5.00E+01	1.05E+01	3.85E+01	2.60E-02	6.00E+03	3.48E-02	1.28E-01	7.84E+00
6.00E+01	6.47E+00	2.37E+01	4.21E-02	7.00E+03	3.52E-02	1.29E-01	7.75E+00
7.00E+01	4.28E+00	1.57E+01	6.37E-02	8.00E+03	3.58E-02	1.31E-01	7.63E+00
8.00E+01	3.02E+00	1.11E+01	9.04E-02	9.00E+03	3.64E-02	1.34E-01	7.48E+00
9.00E+01	2.20E+00	8.08E+00	1.24E-01	1.00E+04	3.72E-02	1.36E-01	7.33E+00
1.00E+02	1.67E+00	6.13E+00	1.63E-01				

low-range of photon energies. This is due to the fact that these γ-rays have correspondingly large value of total attenuation coefficient (μ) for NaI(Tl) and therefore even small thickness is sufficient to absorb all of incident photons. However, for higher values of photon energies, the corresponding value of total attenuation coefficient becomes smaller and as a result there is considerable transmission through relatively thin detectors which leads to smaller values of total efficiencies. This fact can clearly be seen in the 5 MeV energy range where a 1" thick detector has the smallest total efficiency while 10" detector has the highest value. It is also noticeable that in the high energy range, the values of total efficiency tend to saturate to a maximum values as the detector thickness is increased.

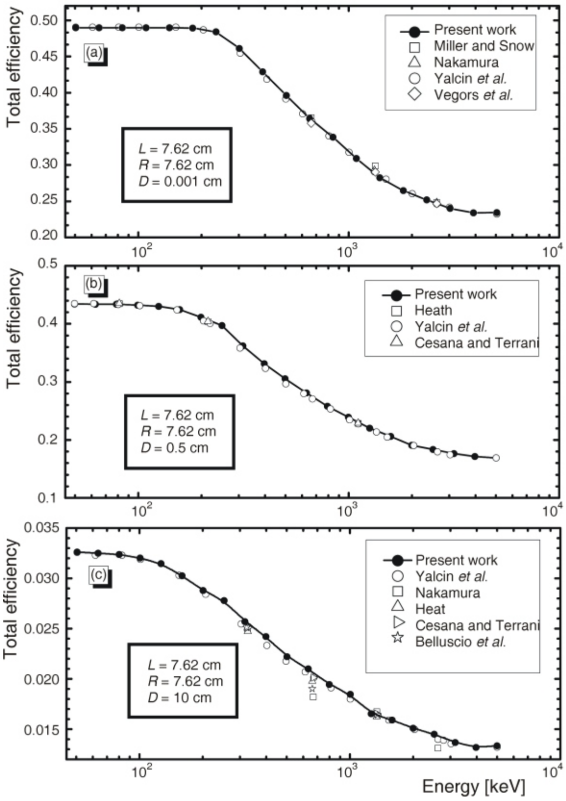

Figure 3. Comparison of total detection efficiency for a 3" 3" NaI(Tl) detector with -ray energy with corresponding hybrid Monte Carlo, direct and experimental results for various values of axial source to detector distance (a) *D* = 0.001 cm, (b) *D* = 0.5 cm, and (c) *D* = 10 cm

The dependence of total efficiency on the detector diameter has also been studied using BPIMC program. The source has been considered at 5 cm axial distance from the front face of a 3" thick cylindrical NaI(Tl) detector. The detector radius has been increased from one inch to 10 inches and in each case energy dependent total efficiency profile has been calculated using BPIMC program. These results are shown in fig. 7.

As the detector radius is increased, the solid angle between source and detector increases which leads to increase in the number of intercepted photons. As a consequence, total efficiency should increase by increasing detector radius. The calculated values of BPIMC code are consistent with this expected behavior. For a 10 inch detector radius, the maximum total detector efficiency is found to approach 0.4. It is also observed that the incremental rise in the values of total efficiency for the same step increase in detector radius becomes smaller and smaller as the detector radius increases, which indicates that for detectors having very large radii, total efficiency is expected to approach certain maximum value.

CONCLUSIONS

The proposed primary-interaction Monte Carlo methodology has been found to yield comparable re-

Table 2. Values of total efficiency of the 3" 3" cylinderical NaI(Tl) detector at various γ-ray energies at indicated values of axial distances *D*

Energy [keV]	Total efficiency					
D = 0.001 cm	Present work	Yalcin *et al.* (2007) [35]	Nakamura (1972) [42]	Miller and Snow (1961) [17]	Vegors *et al.* (1958) [37]	–
661	0.3737	0.3646	0.367	0.370	0.362	–
1332	0.2974	0.2930	0.296	0.302	0.293	–
2620	0.2495	0.2476	0.249	0.250	0.248	–
D = 0.5 cm	Present work	Yalcin *et al.* (2007) [35]	Cesana and Terrani (1977) [39]	Heath (1964) [38]	–	–
80	0.4330	0.4333	0.435	0.435	–	–
212	0.4078	0.4013	0.404	0.403	–	–
110	0.2313	0.2281	0.229	0.228	–	–
D = 10 cm	Present work	Yalcin *et al.* (2007) [35]	Cesana and Terrani (1964) [39]	Heath (1964) [38]	Belluscio *et al.* (1974) [41]	Nakamura (1972) [42]
320	0.0255	0.0249	0.0251	0.0247	0.0250	–
662	0.0207	0.0202	0.0201	0.0198	0.0190	0.0183
1332	0.0169	0.0164	0.0165	0.0162	0.0164	0.0168
2620	0.0142	0.0140	–	–	–	0.0132
2750	0.0140	0.0139	–	–	0.0141	–

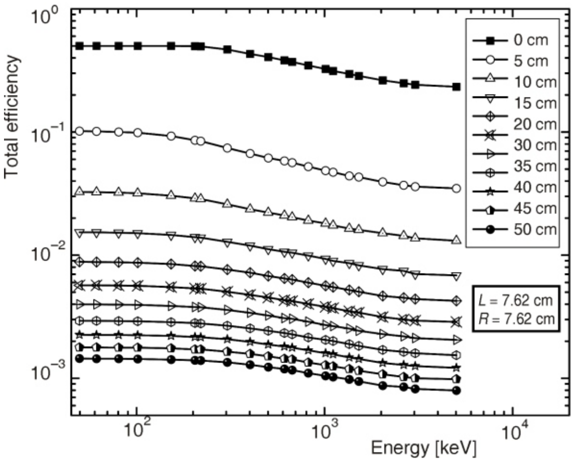

Figure 4. Variation of total detection efficiency for a 3" 3" NaI(Tl) detector with -ray energy for various indicated values of axial source-to-detector distance *D*

sults to those found by direct, hybrid Monte Carlo, standard Monte Carlo, as well as by experimental methods. It converges quickly, reducing standard deviations to less than about 0.4% in only 10^4 histories in contrast with 10^6 required by a hybrid Monte Carlo method. High computational efficiency of BPIMC code stems from the usage of biasing in these Monte Carlo simulations along with primary interaction based scoring technique.

The proposed methodology is flexible and has been extended from axially to non-axially located point isotropic sources where, again, the predictions of BPIMC code have been found in good agreement with direct, theoretical, as well as experimental methods. This indicates the capability of the proposed methodology for handling complex geometries with relative ease. Finally, this methodology has been used for the study of the dependence of total efficiency on the detector thickness and radius. The BPIMC results have been found consistent with the expected behavior for these cases.

Table 3. Comparison of BPIMC calculated values of total efficiency for E_γ = 0.662 MeV at various indicated distances with the corresponding values obtained by using direct, theoretical and experimental methods

ρ [cm]	*D* [cm]	$\varepsilon_{tot}(10^4)$		Normalized values			
		Present work	Selim & Abbas (1996) [40]	Present work	Selim & Abbas (1996) [40]	Beam *et al.* (1978) [28]	
						Experiment	Theory
0.0	45.0	5.6125	5.5500	1.0	1.0	1.0	1.0
22.5	39.0	6.0561	6.3089	1.079	1.1367	1.136	1.057
31.8	31.8	6.3048	6.6282	1.124	1.1947	1.201	1.123
39.0	22.5	6.5261	6.8356	1.163	1.2316	1.276	1.172
45.0	0.0	6.7231	7.3519	1.198	1.3247	1.320	1.220
0.0	15.0	4.3165	4.2790	1.0	1.0	1.0	1.0
7.5	13.0	4.5530	4.6980	1.055	1.0979	1.051	1.034
10.6	10.6	4.8605	4.9972	1.126	1.1679	1.151	1.099
13.0	7.5	5.2049	5.3233	1.206	1.2441	1.244	1.215
15.0	0.0	5.9802	5.9325	1.386	1.3864	1.557	1.414

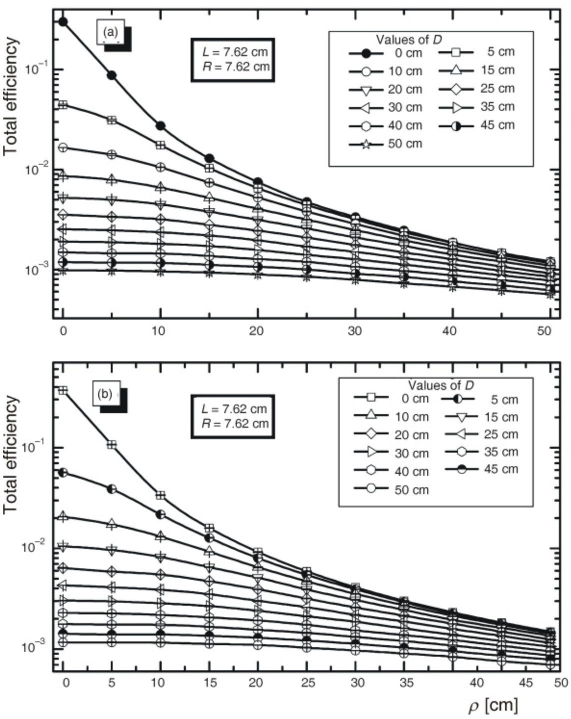

Figure 5. Variation of total detection efficiency for a 3" 3" in NaI(Tl) detector with axial off-set distance for various indicated values of axial source-to-detector distance *D*, (a) for ^{60}Co and (b) for ^{137}Cs sources

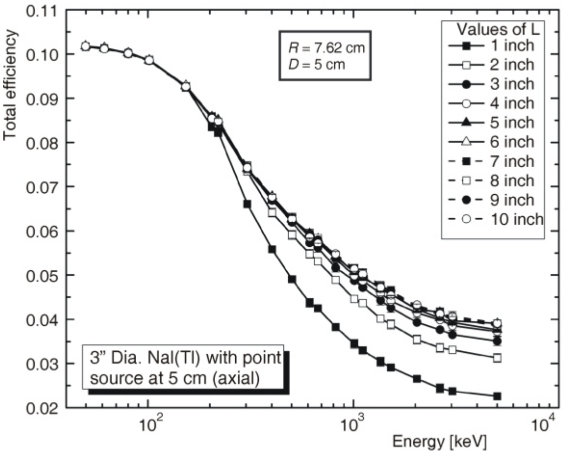

Figure 6. Variation of total detection efficiency for a cylindrical NaI(Tl) detector, having 3" diameter, with -ray energy for indicated values of the detector thickness *L*

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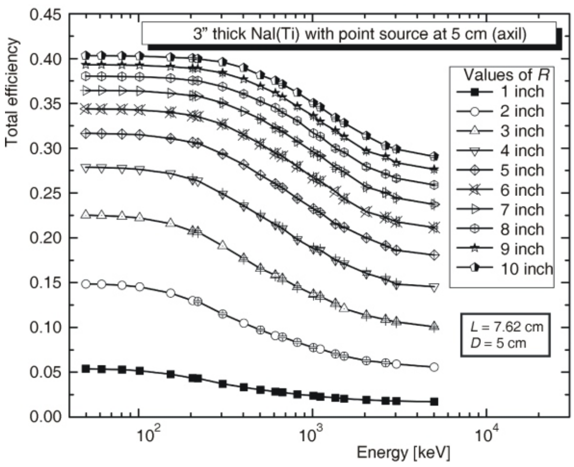

Figure 7. Variation of total detection efficiency for a cylindrical NaI(Tl) detector, having 3" thickness, with -ray energy for indicated values of the detector radius

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ЈЕДАН МОНТЕ КАРЛО ПОСТУПАК ЗА БРЗО ОДРЕЂИВАЊЕ УКУПНЕ ЕФИКАСНОСТИ ЦИЛИНДРИЧНОГ СЦИНТИЛАЦИОНОГ ГАМА ДЕТЕКТОРА

Ради одређивања укупне ефикасности цилиндричног сцинтилационог детектора гама зрачења, развијен је Монте Карло алгоритам заснован на примарној интеракцији. Овај поступак уграђен је у BPIMC рачунарски програм на Матлаб основи. За тачкасте изотропне изворе смештене аксијално у односу на осу детектора, предвиђања добијена BPIMC кодом и одговарајући резултати хибридне Монте Карло методе, као и експериментална мерења у широком распону енергија гама зрачења, сложила су се веома добро. За тачкасте изворе удаљене од аксијалне осе, поређење предвиђања BPIMC кода са одговарајућим резултатима добијеним директним прорачунима или уобичајеним Монте Карло процедурама, добро се слажу – потврђујући тиме предложени алгоритам. Коришћењем BPIMC кода утврђено је да енергетска зависност детекторске ефикасности добија асимптотски облик са повећањем дебљине или пречника сцинтилатора при фиксним осталим вредностима. Програмом BPIMC проучавана је промена енергетске зависности укупне ефикасности 3" 3" Nal(Tl) сцинтилатора у аксијалном правцу. При варијацији аксијалног растојања од 0 cm до 50 cm, примећена је промена око два реда величине у детекторској ефикасности. За ^{137}Cs и ^{60}Co изворе при малим вредностима аксијалног одступања, такође је уочена велика промена укупне ефикасности са порастом аксијалног растојања од 0 cm до 50 cm.

Кључне речи: сцинтилациони детектор, укупна ефикасност, тачкасти извор, Монте Карло симулација