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Limitations in the PHOTON Monte Carlo gamma transport code

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Abstract

Three Monte Carlo gamma transport codes, MCNP, EGS, PHOTON, differ in the degree of difficulty in implementing them for calculation and in the requirements for the input file. Differences in the results were discovered when evaluating the same case using these three transport codes. These differences that are energy dependent are presented here. © 2002 Published by Elsevier Science B.V.

PHOTON is a newly developed, user-friendly, Monte Carlo gamma transport code that was published recently [1]. PHOTON uses a simplified input-file structure wherein the system and the source are described using combinatorial geometry; it also contains its own build-in cross-sectional libraries. However, at low photon energies (<100 keV), care must be exercised in using it since Rayleigh scattering, fluorescence yields, form factors, and scattering factors are not included in the cross-section libraries. Since they cannot presently be included in the libraries, unless the code is modified, at low energies this might limit the code's usefulness. At energies above 1 MeV, we detected systematic discrepancies between the PHOTON code and two well-established Monte Carlo photon-transport codes, MCNP4B [2] and EGS4 [3], when calculating energy deposition spectra in a NaI detector. These discrepancies, that were found to be energy-dependent, are discussed in this communication.

We calculated energy-deposition spectra in NaI (Tl) detectors varying in size using PHOTON code at incident photon energies in the range from 1 to 10 MeV. An input file for the PHOTON code consisted of a point source on the central axis of a cylindrical detector placed 10 cm away from its front face. The energy-deposition spectra (not the pulse height distributions) were calculated for an isotropic point source in which the emitted radiation was limited by the solid angle subtended by the detector, and the space outside the detector was assumed to be in a vacuum [4]. The energy spectra were calculated using 512 channels 20 keV wide. Since no experiments were planned, these calculations were verified with independent calculations using the MCNP4B and EGS4 codes. For this purpose, identical input files were prepared for the other two codes and the calculations were carried out for 10^6 histories. It was noticed that the execution times, for 4.4 MeV gamma rays on a Pentium P166 PC, using PHOTON, MCNP4B,

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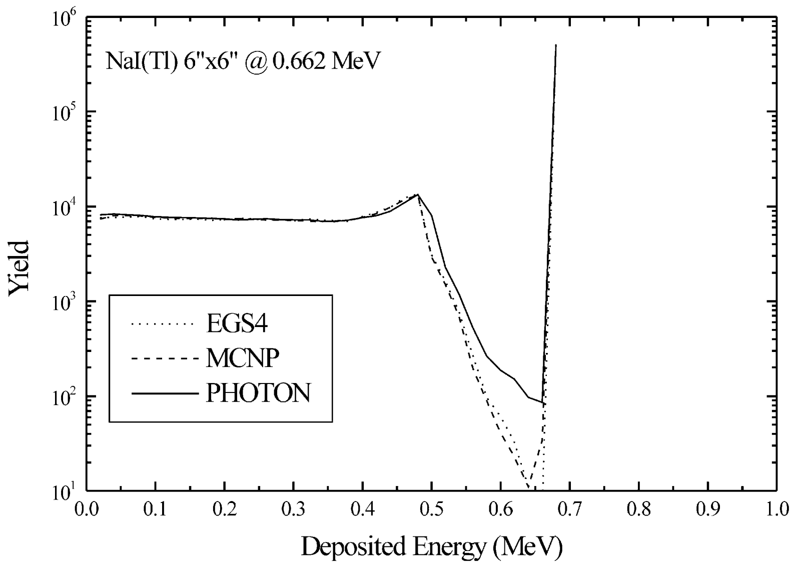

Fig. 1. Energy deposition into a $6'' \times 6''$ NaI detector from a 0.662 MeV point source calculated by the PHOTON, MCNP4B2, and EGS4 Monte Carlo transport codes.

and EGS4 codes were 35 min, 6 min, and about 4 h, respectively. The long computing time for the EGS4 code is due to its treatment of electron-transport using an analog Monte Carlo scheme, not present in the other two codes.

The results reported here represent calculations only for a single size ($6'' \times 6''$) detector. Fig. 1 shows the calculated energy spectra obtained from all three codes at 0.662 MeV. In general, these spectra are in a good agreement except in the valley region on the low-energy side of the photopeak. This discrepancy is partially attributed to the differences in the energy cut-off used in each one of the codes to terminate the particle history, which in the PHOTON code is higher, and, in part, to the different step-sizes used in each of the transport codes. Changing the cut-off energy affected the degree of the discrepancy in this region of the spectrum. However, the discrepancy reported here occurs at higher incident energies.

At energies above 0.662 MeV, energy spectra were calculated at 2, 4.4, 6, 8, and 10 MeV. Only two spectra, corresponding to carbon photopeak, at 4.4 MeV, and in the vicinity of the 9.17 MeV nitrogen peak, at 10 MeV, are shown in Figs. 2a and 3a, respectively. While there is a general agreement between the MCNP4B and EGS4 results, there is a clear discrepancy between these two codes and the PHOTON calculations. This discrepancy increases systematically with the increase in the energy of the incident gamma radiation (Figs. 2a and 3a). Similar discrepancies were apparent in the energy spectra calculated for different detector sizes, not shown here. The missing energy deposition in the PHOTON code, and at the same time higher photopeak yields (see Table 1), have been attributed to the omission of the contribution to the energy spectra from bremsstrahlung radiation, due to electrons and positrons, that results from photoelectric-, Compton-, and pair-production interactions in the detector. To confirm this hypothesis an MCNP code was modified to turn off the production of bremsstrahlung radiation in the detector. These results showed a significant improvement in the agreement between the PHOTON code and the modified MCNP4B code at all incident photon energies; these improvements at 4.4 and 10 MeV are shown in Figs. 2b and 3b, respectively. No change in the spectrum was observed at 0.662 MeV at which the contribution of bremsstrahlung is negligible. Table 1 summarizes yields at the

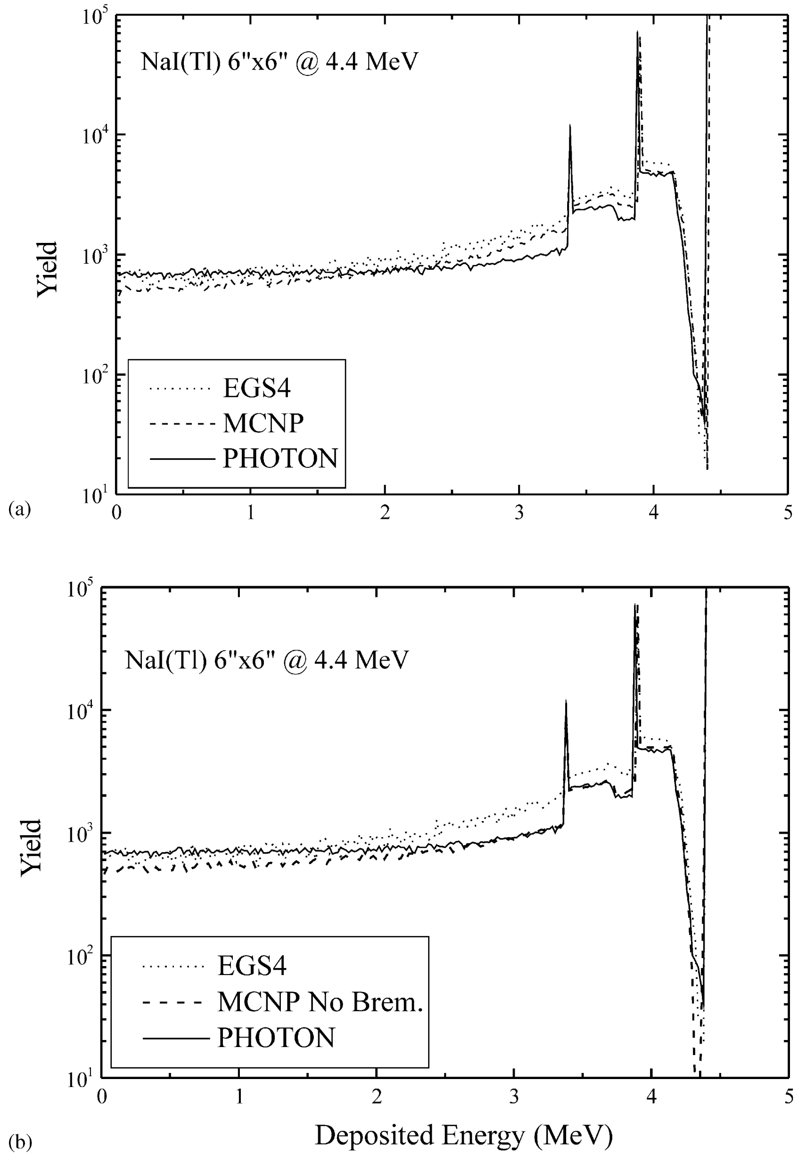

Fig. 2. Comparison of the results obtained from PHOTON, MCNP4B2, and EGS4 Monte Carlo codes at 4.4 MeV: (a) with bremsstrahlung; (b) without bremsstrahlung, demonstrates the effect of the bremsstrahlung contribution.

photopeak (PP), the escape-peak (EP), and double-escape-peak (DE) for all the cases discussed above. It is pointed out that in those applications where only the intensity of the total absorption photpeak is of interest, PHOTON code can be quite useful up to about 4 MeV at which inclusion or exclusion of the bremsstrahlung processes makes a difference of about 10%. However, this difference is energy-dependent and increases with the increase in the incident energy of the gamma rays.

In Monte Carlo calculations, some differences in the simulated spectra are always expected due to the statistical nature of the calculations. However, these differences will tend to decrease with improvements in the calculations. Further

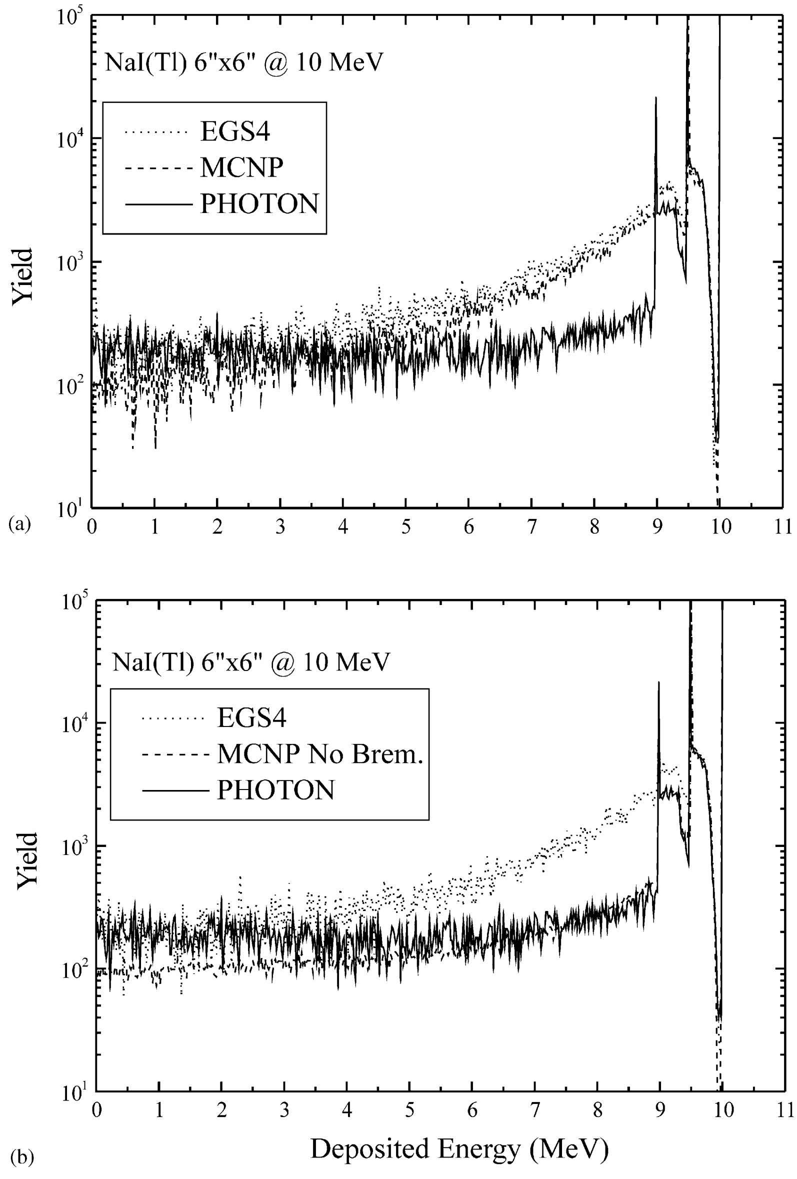

Fig. 3. Comparison of the results of PHOTON, MCNP4B2, and EGS4 Monte Carlo codes at 10.0 MeV: (a) with bremsstrahlung; (b) without bremsstrahlung, demonstrates the effect of the bremsstrahlung contribution.

discrepancies of several percent may arise in the calculations due to the different cross-section libraries used in each code: XCOM for PHOTON [5]; MCPLIB02 for MCNP4B [6]; and, PEGS4 for EGS4 [3]. For example, Table 2 shows the total mass attenuation coefficients at three energies derived from the cross-sections used in each of codes. At 1 MeV there is 2.5% difference in the total mass attenuation coefficients and it grows to about 7% at 10 MeV.

Due to the effects observed, in the energy region where the discrepancy occurs and the intensities of the escape peaks, it was suspected that the bremsstrahlung process is responsible for the effect. The bremsstrahlung cross-sections are calculated separately for two energy ranges, one

Table 1
Normalized yield per history of the photopeak (PP), single-escape (SE) peak, and double-escape (DE) peaks, obtained from the calculations with PHOTON, EGS4, MCNP4B, and MCNP4B with bremsstrahlung turned-off[a].

E (MeV)	PHOTON			EGS4			MCNP4B			MCNP4B-No Brem.		
	PP	SE	DE	PP	SE	DE	PP	SE	DE	PP	SE	DE
0.662	0.5013	—	—	0.5061	—	—	0.5069	—	—	0.5082	—	—
2.000	0.2702	0.0146	0.0022	0.3045	0.0145	0.0018	0.2716	0.0139	0.0018	0.2801	0.0123	0.0019
4.400	0.1919	0.0601	0.0083	0.2086	0.0573	0.0058	0.1823	0.0554	0.0068	0.2040	0.0609	0.0071
	0.2%	(0.3%)	(1.0%)	(0.2%)	(0.4%)	(1.3%)	(0.2%)	(0.4%)	(1.2%)	(0.2%)	(0.4%)	(1.2%)
6.000	0.1689	0.0932	0.0134	0.1586	0.0720	0.0063	0.1465	0.0742	0.0087	0.1816	0.0945	0.0123
8.000	0.1600	0.1174	0.0167	0.1319	0.0753	0.0068	0.1240	0.0790	0.0089	0.1732	0.1178	0.0155
10.00	0.1567	0.1356	0.0195	0.1173	0.080	0.0089	0.1076	0.0780	0.0085	0.1712	0.1381	0.0186
	(0.2%)	(0.3%)	(0.7%)	(0.1%)	(0.2%)	(1.3%)	(0.3%)	(0.3%)	(1.1%)	(0.2%)	(0.3%)	(0.7%)

[a] In all cases, 10^6 histories were executed. The SDs in parentheses are shown only at 4.4 and 10 MeV; all the others were very similar in magnitude

Table 2
Total mass attenuation coefficients (cm^2/g) in a NaI detector at three different energies

Energy (MeV)	MCPLIB02 (MCNP4B)	PEGS4 (EGS4)	XCOM (PHOTON)
0.10	1.679×10^{-0}	1.657×10^{-0}	1.669×10^{-0}
1.00	5.911×10^{-2}	5.876×10^{-2}	5.762×10^{-2}
10.0	3.934×10^{-2}	3.674×10^{-2}	3.722×10^{-2}

below 2 MeV, and the other above 50 MeV; the cross-sections for the intermediate range, of 2–50 MeV, are interpolated [7]. Thus, a library can be written that contains these cross-sections up to 10 MeV based on interpolations. However, the cross-sections for electron–photon energy transfer will not be predicted correctly, as shown in Fig. 6 of Ref. [7], if they are based only on extrapolation from the equation for cross-sections at low energies. The comparison of the PHOTON spectral shape and the yields of the peaks with the results of the MCNP4B code without bremsstrahlung showed a significant improvement in their agreement, although there are still differences in the low-energy part of the spectra. Thus the need to include proper bremsstrahlung production processes in the PHOTON code has been recognized. Inclusion of bremsstrahlung will make the PHOTON code much more reliable at higher energies. However, the authors feel that the real drawback of the code, in its current version, is the inability to modify its cross-sections.

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