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General Formalism for Calculating Gamma-Ray Buildup Factors in Multilayer Shields into MERCURE-6 Code

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This study proposes a new method for calculating gamma-ray buildup factors in multilayer shields. The formula combines the buildup of single-layer shields with products and quotients. The tests have shown that the approximating formula reproduces the reference data of double layer shields very well for most cases. With the same parameters and with a new physical consideration that takes into account in a global way the degradation of the gamma-ray energy spectrum, the buildup factors of three and five layer shields were also very well reproduced. The new formula is incorporated in the new version of the MERCURE-6 point-kernel code.

KEYWORDS: gamma-ray buildup factors, energy range 40 keV-10 MeV, fluorescence, bremsstrahlung, coherent and incoherent scattering, point isotropic source, multilayer shields, comparative evaluations, SN1D code, MERCURE-6 code

I. Introduction

The calculation of gamma-ray attenuation through single or multilayer shields can be performed by solving rigorously the Boltzmann transport equation by a deterministic method (discrete ordinates method), or by a probabilistic method (Monte-Carlo method). However, this approach is not always practical in shielding design because of the need for sophisticated computer codes and long computer time [1].

For project or pre-project studies, the attenuation of gamma rays is usually estimated by simpler and faster methods, such as the point kernel calculation method, implemented in MERCURE-5 and QAD codes (Refs. 2 and 3, respectively), for example, incorporating gamma-ray buildup factors. The gamma-ray buildup factors of multilayer shields must be represented in the point-kernel codes by an empirical formula in terms of buildup factors of single layer shields with parameters determined by fitting the reference data from rigorous and accurate calculations.

Recently, the authors have proposed a new empirical formula[4, 5], starting initially from the study of Harima et al.[6], for calculating gamma ray buildup factors in multilayer shields. The formula combines the buildup factors of single layer shields with products and quotients. The feasibility of the formula for reproducing the buildup factors was tested by using point isotropic buildup factors calculated with the SN1D discrete ordinates code as reference data[7]. The dose buildup factors of single, double, and multilayer shields composed of water, aluminum, iron and lead were calculated for a spherical geometry in the energy range between 10 MeV and 40 keV and for total thicknesses of up to 30 mean free paths (mfp).

In this paper the formula and new gamma-ray libraries of single layer buildup factors and cross sections are incorporated in the new version of the MERCURE-6 point-kernel code. The dose rates calculated by MERCURE-6 are compared with those obtained from rigorous transport calculations performed by the discrete ordinates code SN1D[8]. The comparisons are presented for multilayer shields composed of water, iron, and lead, for 4 energies of 10, 1, 0.511, and 0.04 MeV, and for total thicknesses of up to 30 mean free paths.

II. Reference Data Calculations

The reference data calculations were performed by using the SN1D discrete ordinates code, with general anisotropic scattering [i.e., an L'th order (P_L) Legendre expansion of the scattering cross sections]. The SN1D code, which was developed at the Commissariat à l'Energie Atomique (CEA), Saclay, is analogous to the ANISN code[9]. It solves the one dimensional Boltzmann transport equation for slab, cylindrical, or spherical geometry; the cross sections are averaged in an energy group structure.

The dose rates were calculated in three and five layer shields composed of water, iron and lead, for a spherical geometry with a point isotropic source represented in the SN1D transport calculations by a sphere with radius equal to 0.01 mfp of the energy source group. The dose rates were determined for 4 energies in the 10 MeV-40 keV energy range and for total thicknesses of up to 30 mfp. The calculations take into account the coherent and incoherent scattering, the pair production, and the secondary sources of bremsstrahlung and fluorescence[10]. The photon cross sections data used were taken from the JEF2[11] compilation and the conversion factors from flux to dose from the ANS-6.1.1-1977 report[12].

The calculation of the dose rates up to 30 mfp shield thickness by the discrete ordinates method is very difficult and needs many energy groups and an extremely fine space and angular mesh to achieve reasonably accurate results[13]. Therefore, the

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dose rates were generated by the SN1D code with the following features: 218 energy groups between 10 MeV and 1 keV for the transport calculations, P_7 for the Legendre expansion of the scattering cross sections and S_{96} for the Gauss-Legendre angular quadrature, 728 spatial meshes between 0 and 35 mfp (1 mfp is divided into 20 subintervals).

III. Approximating Formula for Buildup Factors

1. General Expression of the Formula for Multilayer Shields. Method 1 of Calculation

Consider a multilayer shield composed of N layers of different materials ($N \geq 2$) with X_1 mfp of the first material followed by X_2 mfp of the second material, and X_N mfp of the N'th material. Let $t_1=X_1$, $t_2=X_2+t_1$, $t_N=X_N+t_{N-1}$. The buildup factors recently proposed by the authors are calculated in this multilayer shield by the following equations[7],

$$B(t_1)=B_1(t_1)$$

$$B(t_N)=\frac{B(t_{N-1})}{B_N(t_{N-1})}B_N(t_N)F(X_{N-1};X_N) \quad (1)$$

where

$B(t_N)$ is the buildup factor for the N layer shield composed of X_1 mfp of the first material followed by X_2 mfp of the second material, and X_N mfp of the N'th material,

$B(t_{N-1})$ is the buildup factor for the (N-1) layer shield composed of X_1 mfp of the first material followed by X_2 mfp of the second material, and X_{N-1} mfp of the N-1'st material,

$B_N(t_N)$ is the infinite buildup factor of the N'th material at t_N mfp,

$B_N(t_{N-1})$ is the infinite buildup factor of the N'th material at t_{N-1} mfp,

$F(X_{N-1};X_N)$ is a fitting function that depends on X_{N-1} and X_N.

The function $F(X_{N-1};X_N)$ is given by

$$F(X_{N-1},X_N)=\left[\frac{\alpha_{N-1,N}+X_N{}^{\beta_{N-1,N}}}{\alpha_{N-1,N}}\right]^p \quad (2)$$

with

$$\log(\alpha_{N-1,N})=a\log^2(X_{N-1})+b\log(X_{N-1})+c$$

and (3)

$$\log(\beta_{N-1,N})=d\log(X_{N-1})+e$$

where a, b, c, d and e are five parameters that depend on the energy source and the materials considered as well as on their arrangement in the multilayer shield. The parameter p is a function of the energy source and the shield combinations. It takes three values (p=-1,0,1). The parameters a, b, c, d, e, and p were calculated for 10 double layer shields composed of water, aluminum, iron, and lead. Their values are listed in Ref. 7 for the water-iron, iron-water, water-lead and lead-water shields at 10, 3, 1, 0.511, 0.1, and 0.04 MeV.

Equations (1), (2) and (3) are applied to a multilayer shield of N layers by considering the first (N-1) layers as a single layer composed of the (N-1'st) materials. Then, the buildup factors of this (N-1) layer shields are calculated by applying the equations to a double layer shield of (N-2) layers followed by the (N-1'st) layer and so on.

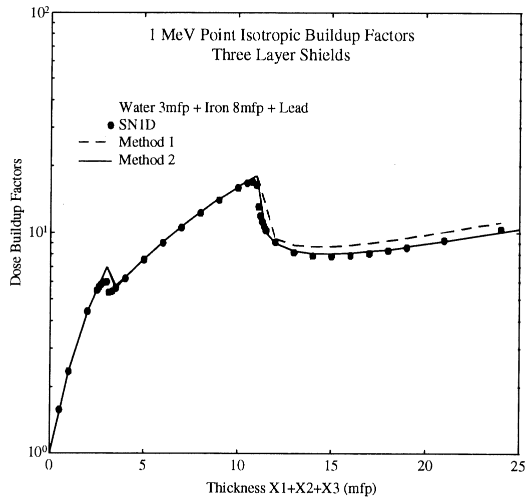

Fig. 1 Point isotropic buildup factors for three-layer shields of 3 mfp of water followed by 8 mfp of iron and 14 mfp of lead at 1 MeV.

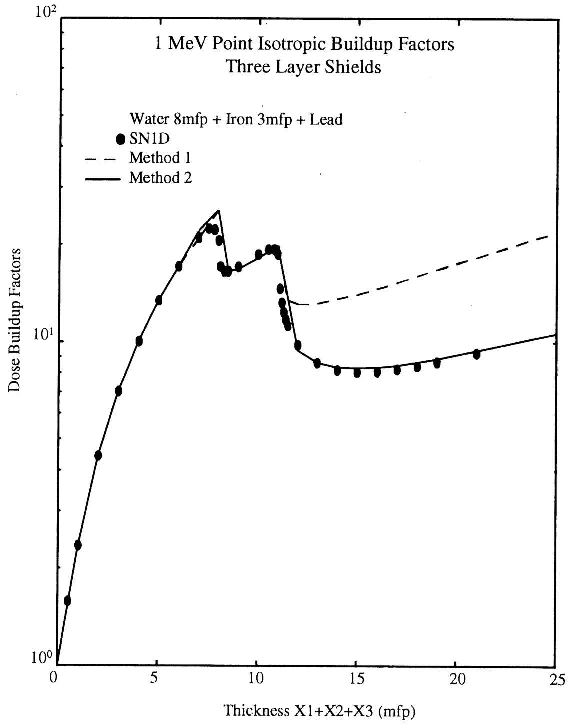

Fig. 2 Point isotropic buildup factors for three-layer shields of 8 mfp of water followed by 3 mfp of iron and 14 mfp of lead at 1 MeV.

Figure 1 shows the dose buildup factors for three layer shields composed of 3 mfp of water followed by 8 mfp of iron and 14 mfp of lead, as a function of the total thickness $X_1+X_2+X_3$ of the three materials, for a 1 MeV point isotropic source. The discontinuous curve represents the reference data calculated by the SN1D code, and the dashed curve (method 1) the data obtained by equations (1), (2) and (3) using the parameters determined for the water-iron and the iron-lead shields at 1 MeV. As seen in Fig. 1, the approximating formula reproduces very well the reference data. The maximum deviations observed are~10%.

Figure 2 shows the dose buildup factors for the same three layer shields, but with 8 mfp of water followed by 3 mfp of iron and 14 mfp of lead. In this case, the approximating formula overestimates the buildup factors in the lead shield by a factor of ~2. These large deviations are explained by the fact that the parameters determined for the iron-lead shield at 1 MeV are not applicable anymore because of the degradation of the gamma ray energy spectrum in the first 8 mfp water shield. The energies of the gamma rays traversing 8 mfp of water are lower than the source energy. Therefore, the method 1 of calculation does not always reproduce accurately the buildup factors in multilayer shields composed of materials of large thicknesses.

2. General Expression of the Formula for Multilayer Shields. Method 2 of Calculation

The second method of calculation rests on a new physical consideration that takes into account in a global way, the degradation of the gamma ray energy spectrum in each material traversed. In this method, the N layer shield is divided into (N-1) two layer shields, and the total thickness of each double layer shield is replaced by an equivalent thickness of the second material. The buildup factors are calculated by Eqs. (1), (2), and (3) for each double layer shield.

For example, the buildup factors of a three layer shield composed of X_1 mfp of water followed by X_2 mfp of iron and X_3 mfp of lead are calculated by first applying Eqs. (1), (2), and (3) for a double layer shield composed of X_1 mfp of water followed by X_2 mfp of iron. Then, from the result of this calculation, an equivalent thickness X' of iron is determined, and the buildup factors in the iron-lead shield are calculated by the same equations but with X' mfp of iron followed by X_3 mfp of lead.

The equivalent thickness X' is given by the following formula,

$$B(X_1+X_2)=\frac{B_1(X_1)}{B_2(X_1)}B_2(X_1+X_2)F(X_1;X_2)=B(X')$$

and (4)

$$B(X'+X_3)=\frac{B_2(X')}{B_3(X')}B_3(X'+X_3)F(X';X_3)=B(X'')$$

The solid curve of figure 2 (method 2) represents the dose buildup factors in the water-iron-lead shield calculated using this method. As seen in Fig. 2, the approximating formula reproduces very well the reference data. The maximum deviations observed in the lead shield are within 10%.

IV. Comparison MERCURE-6/SN1D

The formula using the second method of calculation has been incorporated in the new version of the MERCURE-6 point-kernel code developed at CEA (Saclay France). The MERCURE-6 is a direct line-of-sight point kernel code which makes quick calculations of dose rates and exposures in 3 dimensional geometry. The total response from a point source is obtained by integrating the kernel over the source volume by a Monte-Carlo technique. To be coherent with the SN1D transport calculations, new gamma-ray libraries of single layer buildup factors and cross sections were integrated in MERCURE-6 in a 195 energy-group-structure. The 195 energy-group-structure is identical to the 218 energy-group-structure between 10 MeV and 40 keV.

Figures 3, 4, and **5** show the dose rates in three layer shields composed of water, iron, and lead at 10, 1, 0.511, and 0.04 MeV. The solid curves represent the reference data calculated by SN1D and the discontinuous curves the data obtained by MERCURE-6. As seen in this figure, the dose rates calculated by MERCURE-6 are in very good agreement with those obtained by SN1D for most cases. At 1 and 0.511 MeV, the maximum deviations observed between the two codes are within 15% at 20 mfp in both the water-iron-lead and the iron-water-lead shields (Figs. 3 and 4). These deviations become ~25% and ~20% at 20 mfp in the iron-lead-water shield at 1 and 0.511 MeV respectively (Fig. 5). At 10 MeV, the maximum deviations observed at 20 mfp are ~25% and ~5% in the water-iron-lead and the iron-water-lead shields respectively. However, in the iron-lead-water shield the dose rates are underestimated by 38% at 20 mfp. At 0.04 MeV, the maximum deviations observed at 20 mfp in the water-iron-lead, iron-water-lead, and iron-lead-water shields are about 20%, 16%, and 25% respectively. It is important to note that all the deviations observed between SN1D and MERCURE-6 correspond to those seen in Ref. 7 for the double layer buildup factors. Thus the method 2 of calculation induces no additional errors and takes into account in a global way the degradation of the gamma-rays energy spectrum. Moreover, the large deviations observed in some cases are acceptable because they occur only at very deep penetrations (250 cm to 700 cm).

Figure 6 shows the dose rates in five layer shields composed of 8 mfp of water followed by 2 mfp of iron, 10 mfp of lead, 8 mfp of water and 2mfp of iron, at 10, 1, 0.511, and 0.04 MeV. The continuous curve represents the data obtained by SN1D and the discontinuous curve the data obtained by MERCURE-6 using the second method of calculation. The maximum deviations observed at very deep penetrations (30 mfp) are about 22%, 20%, 14%, and 73% at 10, 1, 0.511, and 0.04 MeV respectively. The 73% overestimation observed at 0.04 MeV is not representation of any weakness in the method but is due to the lack of information on the library which requires an extrapolation. This example shows that the formula reproduces the buildup factors in multilayer shields composed of a great number of layers with strong attenuation in a wide range of energy.

V. Conclusions

A new approximating formula for calculating the gamma ray buildup factors in multilayer shields was proposed. The formula combines the buildup factors of single layer shields with products and quotients.

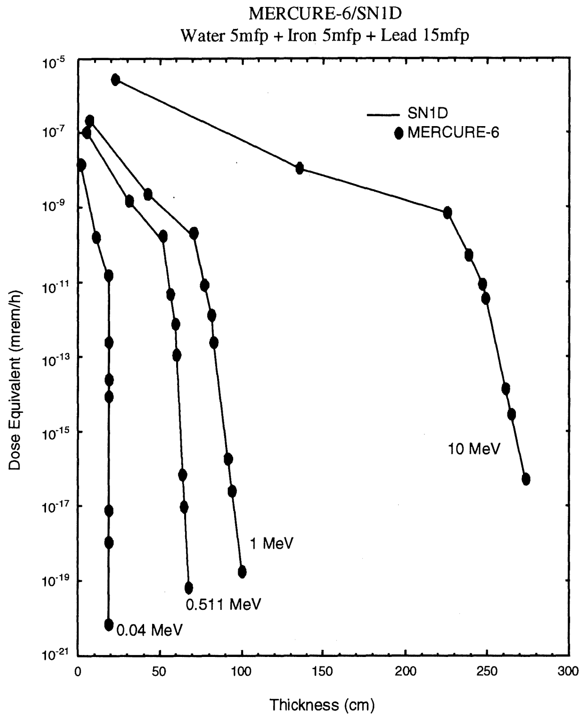

Fig. 3 Dose rates for three-layer shields of 5 mfp of water followed by 5 mfp of iron and 14 mfp of lead at 10, 1, 0.511 and 0.04 MeV.

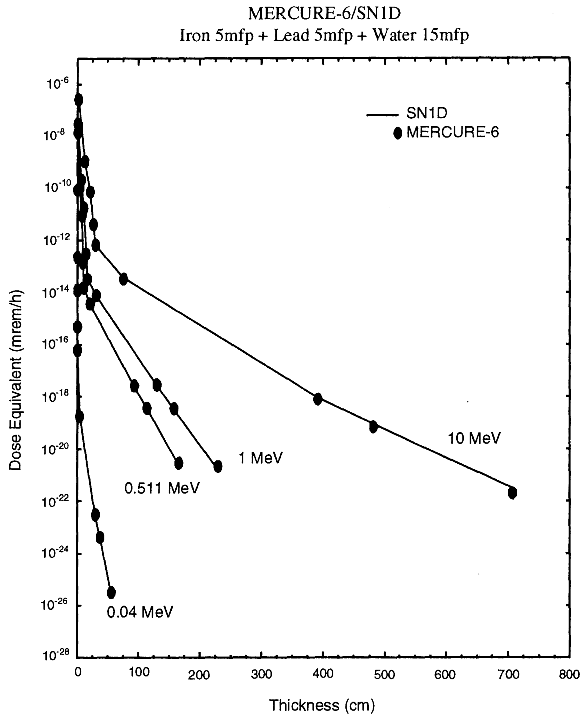

Fig. 5 Dose rates for three-layer shields of 5 mfp of iron followed by 5 mfp of lead and 14 mfp of water at 10, 1, 0.511 and 0.04 MeV.

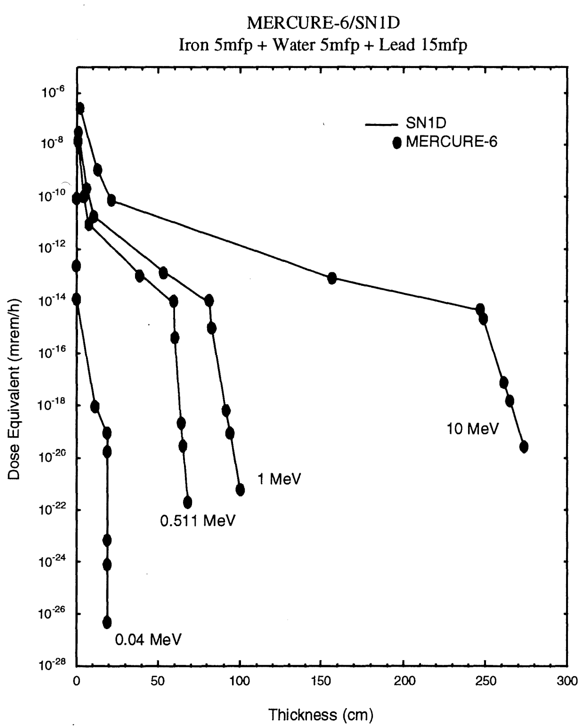

Fig. 4 Dose rates for three-layer shields of 5 mfp of iron followed by 5 mfp of water and 14 mfp of lead at 10, 1, 0.511 and 0.04 MeV.

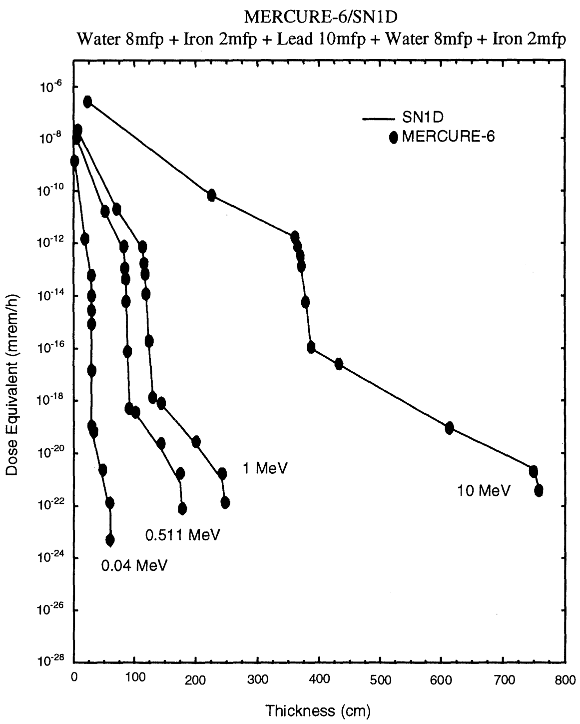

Fig. 6 Dose rates as for five-layer shields at 10, 1, 0.511 and 0.04 MeV.

The formula was already tested and validated by using a new set of point isotropic buildup factors calculated with the SN1D discrete ordinates code as reference data. The dose buildup factors of single, double, and multilayer shields composed of water, aluminum, iron and lead were calculated for a spherical geometry, in the energy range between 10 MeV and 40 keV, and for total thicknesses of up to 30 mfp (mean free path). The calculation of the buildup factors takes into account the bound electron effect of Compton scattering (incoherent scattering), the coherent scattering, the pair production, and the secondary sources of bremsstrahlung and fluorescence.

The test have shown that formula reproduces the buildup factors of double layer shields very well. With the same parameters and with a new physical consideration that takes into account, in a global way, the degradation of the gamma rays energy spectrum, the buildup factors of multilayer shields were also very well reproduced. The large deviations observed in some cases at particular energies are acceptable as an approximating formula and because they occur only at deep penetrations (attenuation $\sim 10^{-10}$).

The advantage of the new formula over all other proposed formulas is that it reproduces the buildup factors of multilayer shields in a wide range of energy $(0.04 \leq E \leq 10\ \text{MeV})$, for thicknesses of up to 30 mfp.

The formula and new gamma-ray libraries of buildup factors and cross have been incorporated in the new version MERCURE-6 point kernel code. The dose rates calculated by MERCURE-6 are in very good agreement with those obtained from rigorous and accurate calculations performed by the SN1D discrete ordinates code.

— References —

(1) Harima, Y. : *Radiat. Phys. Chem.*, **41**, 631 (1993).

(2) Dupont, C. : MERCURE-5, Internal Report, Centre d'Etudes de Saclay (1995).

(3) Malenfant, R. E. : QAD: A series of Point-Kernel General Purpose Shielding Programs, *LA*-3573, Los Alamos National Laboratory (1966).

(4) Assad, A. : PhD Thesis, University of Paris XI, Orsay (1995). (In French).

(5) Assad, A., Diop, C. M., *et al.* : *Proc. 1998 ANS Radiation Protection and Shielding*, Nashville P.II-277 (1998)

(6) Harima, Y., *et al.* : *Proc. Topl. Mtg. New Horizons in Radiation Shielding*, Pasco, Washington, P.473 (1992).

(7) Assad, A., Chiron, M., Nimal, J. C., Diop, C. M. : *Nucl. Sci. Eng.*,**132**, 203 (1999).

(8) Dejonghe, G., Luneville, L. : "SN1D", *Internal Report*, Centre d'Etudes de Saclay (1993).

(9) Engle, W. W. : "A Users Manual for ANISN", *K*-1693, U.S. Atomic Energy Commission (1967).

(10) Kitsos, S., Diop, C. M., Assad, A., Nimal, J. C. : *Nucl. Sci. Eng.*, **123**, 215 (1996).

(11) Files JEF-2, ENDF-B4 and ENDF-B6, OECD/NEA Data Bank, Nuclear Energy Agency (1991).

(12) "Neutron and Gamma-Ray Flux-to-Dose Rate Factors", American National Standard *ANSI/ANS*-6.1.1-1977.

(13) Kitsos, S., Assad, A., Diop, C. M., Nimal, J. C. : *Nucl. Sci.Eng.*, **117**, 47 (1994).