Journal of NUCLEAR SCIENCE and TECHNOLOGY, Supplement 1, p. 502–506 (March 2000)

A Comparison of Gamma-Ray Buildup Factors for Water, Iron and Lead using Discrete Ordinates, Moments, and Monte Carlo Methods

Ali ASSAD*, Maurice CHIRON*,†, Jean Claude NIMAL* and Cheikh M'backé DIOP*

*Commissariat à l'Énergie Atomique, DRN/DMT/SERMA/LEPP

The aim of this study is to compare point isotropic buildup factors recently calculated by Sn discrete ordinate codes with those obtained by the EGS4 Monte Carlo code and those of the standard data (ANS-6.4.3-1991). The comparisons are presented for the water, iron, and lead exposure buildup factors, for 3 energies of 10, 1, and 0.1 MeV, and for total thicknesses of up to 30 mfp mean free paths. The comparisons have shown that the buildup factors calculated by the Sn and EGS4 codes are in very good agreement. The maximum deviations observed between the results given by these codes are about 10% for all cases. The deviations between the Sn and EGS4 codes on the one hand, and the standard data on the other hand, are about 35% and 20% for the lead exposure buildup factors at 10 MeV and 0.1 MeV respectively. In the second part of the study we show the impact of both coherent and incoherent scattering on the exposure and the exposure buildup factors. These effects are important for the energy range below 1 MeV and must not be neglected in the transport calculations.

KEYWORDS: ***gamma-ray buildup factors, 15 keV-10 MeV energy range, fluorescence, bremsstrahlung, coherent and incoherent scattering, point isotropic source, comparative evaluations, Sn codes, EGS4 code, PALLAS code***

I. Introduction

The gamma-ray buildup factor is a multiplicative factor which corrects the response to uncollided photons so as to include the contribution of scattered photons.(1) Buildup factors are important data implemented in point kernel codes (MERCURE(2), QAD(3)), together with linear attenuation coefficients.

Buildup factors can be measured by experiments or calculated by codes solving rigorously the Boltzmann transport equation. Experiments for obtaining accurate buildup factors in a wide range of energy are generally not easy to set up. Therefore, buildup factors are calculated using different codes (SN1D(4), TWODANT(5), EGS4(6), PALLAS(7)), for the same physical problem, and then compared.

In this paper a new set of point isotropic buildup factors(8) recently calculated by Sn discrete ordinates codes (SN1D(4), TWODANT(5)) are compared with those obtained by Hirayama(9) using the EGS4 Monte Carlo code with a particle splitting technique, and those of the standard data, ANS-6.4.3-1991.(10)

The comparisons were firstly performed by neglecting coherent and incoherent scattering and L X-rays in the Sn transport calculations to be conform with the other calculations. The buildup factors calculated by the Sn codes take into account the secondary sources of bremsstrahlung (no distinction between electrons and positrons), the Compton scattering using the theory of Klein-Nishina for free electrons, the pair production, and the photoelectric effect with K X rays. The ELEGAM-2(8) code has been used to produce gamma-ray multigroup transfer matrices for the Sn codes taking into account all the above physical phenomena without changing the transport codes. The comparisons are presented for the water, iron, and lead exposure buildup factors, for 3 energies of 10, 1, and 0.1 MeV, and for total thicknesses of up to 30 mfp (mean free path).

In the second part of the study, we show the impact of both coherent and incoherent scattering on the exposure buildup factors and the exposures. These effects are important for the energy range below 1 MeV and must not be neglected in the transport calculations.

II. Production of g ray Multigroup Transfer Matrices for Sn Codes

The ELEGAM-2 code has been developed at the Commissariat à l'Énergie Atomique (CEA/Saclay) to produce gamma-ray multigroup transfer matrices for the Sn codes (SN1D, TWODANT), by taking into account: the secondary sources of bremsstrahlung coming from the electrons and positrons of the Compton scattering and the pair production effects (with the multiple scattering theory), the coherent scattering (Rayleigh), the bound-electron effect of Compton scattering (incoherent), the pair production, and the photoelectric effect with emission of K and L X rays secondary sources of fluorescence. It is interesting to notice that no modifications in the Sn transport codes are needed. The photon cross sections data are taken from the JEF2 evaluation(11) that has taken back the (EPDL) compilation.(12)

The coherent and incoherent scattering are rigorously treated by the ELEGAM-2 code using the form factors and incoherent scattering functions of the EPDL compilation.(12) (13) Fluorescence is dealt with by an isotropic multigroup energy transfer; the fine structure of the K and L X rays is exactly

* 91191 Gif-sur-Yvette, France

† Corresponding author, Tel.+33-1-69-08-53-82 Fax.+31-1-69-08-45-72, E-mail: chiron@soleil.serma.cea.fr

taken into account using the radiative transitions and the corresponding emission efficiencies from the Evaluated Atomic Data Library Compilation.[14] Concerning secondary sources of bremsstrahlung, their calculation by ELEGAM-2 is rigorous if we consider that the secondary photons are emitted where the Compton scattering or the pair production effect takes place. In other words, if we neglect the track of the charged particles as they pass through matter. In this case ELEGAM-2 first carries out the energy and angular bremsstrahlung gamma distribution for one electron penetrating a thick target with a given kinetic energy $(e^- \rightarrow \gamma_B)$. The obtained gamma distributions are converted into gamma-gamma Legendre multigroup energy transfer matrices required for the Sn codes. Under the previous hypothesis related to electron and positron track, it is clear that the electromagnetic cascade $(\gamma \rightarrow e^- \rightarrow \gamma_B \rightarrow e^- \rightarrow \gamma_B)$ effect is automatically incorporated in the transport calculations.

More details about the ELEGAM-2 code are given in reference 8.

III. Buildup Factor Calculations

The exposure buildup factors for water, iron, and lead are calculated using Sn discrete ordinates codes (SN1D, TWODANT) for point isotropic sources in infinite spherical geometry. The buildup factors are generated for 3 energies of 10, 1, and 0.1 MeV, and for total thicknesses of up to 30 mfp (mean free path).

The calculation of the buildup factors up to 30 mfp shield thickness by the discrete ordinates codes is very difficult and needs many energy groups and an extremely fine space and angular mesh to achieve reasonably accurate results.[15,16] Therefore, the buildup factors are obtained by the Sn codes 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). The results obtained by the two discrete ordinate codes SN1D and TWODANT are identical.

The water, iron, and lead exposure buildup factors tabulated in the ANS-6.4.3 standard data report were calculated for point isotropic sources using two different codes. Those for water and iron were obtained by the moments method[17] with the Hubbell's compilation (NSRDS-NBS-29)[18] for the photon cross sections. Those for lead were determined by the discrete ordinates code, PALLAS[7], with the PHOTX[19] library.

Recently, Hirayama[9] calculated the point isotropic buildup factors for water, iron, and lead up to 40 mfp using the EGS4 Monte Carlo code with a particle splitting technique. The calculations were performed with the same photon cross section libraries mentioned above.

IV. Comparison with the EGS4 Monte Carlo Code and the Standard Data

1. Comparison without Coherent and Incoherent Scattering

The water, iron, and lead exposure buildup factors calculated by the Sn codes are compared with those obtained by the EGS4 code and those of the standard data in **Tables 1** to **4** for 10, 1, and 0.1 MeV point isotropic sources.

At 10 MeV where the contribution of secondary sources of bremsstrahlung becomes important in high Z materials (iron, lead), the buildup factors calculated by the Sn and EGS4 codes are in very good agreement (table 1). The maximum deviations observed between the results given by these codes are about 1% for the water exposure buildup factors, 5% for the iron exposure buildup factors, and less than 10% for the lead exposure buildup factors. The deviations between the Sn and EGS4 codes on the one hand, and the standard data on the other hand, are about 8, 30, and 35% for the water, iron, and lead exposure buildup factors respectively; the moments method underestimates the water and the iron exposure buildup factors and the discrete ordinates code PALLAS overestimates the lead exposure buildup factors. These tendencies which have been

Table 1 Gamma-Ray Exposure Buildup Factors for Point Isotropic Source (10.0 MeV)

mfp	Water					Iron				
	EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)			EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)	A	B	C	(C/B)	(C/A)
1	1.44	1.37	1.44	**1.05**	**1.00**	1.51	1.33	1.50	**1.13**	**0.99**
7	3.31	3.07	3.30	**1.07**	**1.00**	4.29	3.27	4.17	**1.28**	**0,97**
10	4.16	3.86	4.15	**1.08**	**1.00**	6.14	4.69	6.03	**1.29**	**0.98**
20	6.80	6.38	6.83	**1.07**	**1.00**	15.5	12.3	15.9	**1.30**	**1.03**
30	9.45	8.78	9.33	**1.06**	**0.99**	32.2	25.3	33.8	**1.33**	**1.05**

mfp	Lead				
	EGS4 (PHOTX)	ANS-6.4.3 (PHOTX)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)
1	1.57	1.51	1.51	**1.00**	**0.96**
7	6.24	7.37	5.62	**0.76**	**0.90**
10	12.0	15.4	10.8	**0.70**	**0.90**
20	109.	161.	99.9	**0.62**	**0.92**
30	965.	1.47+3	913.	**0.62**	**0.95**

Table 2 Gamma-Ray Exposure Buildup Factors for Point Isotropic Source (10.0 MeV)-Without Bremsstrahlung

mfp	Water					Iron				
	EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)			EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)	A	B	C	(C/B)	(C/A)
1	1.39	1.37	1.39	**1.01**	**1.00**	1.34	1.33	1.34	**1.01**	**1.00**
7	3.15	3.07	3.14	**1.02**	**1.00**	3.36	3.27	3.36	**1.03**	**1.00**
10	3.99	3.86	3.94	**1.02**	**0.99**	4.79	4.69	4.86	**1.04**	**1.01**
20	6.55	6.38	6.50	**1.02**	**0.99**	12.9	12.3	13.2	**1.07**	**1.02**
30	9.18	8.78	8.88	**1.01**	**0.97**	26.6	25.3	28.6	**1.13**	**1.08**

mfp	Lead				
	EGS4 (PHOTX)	ANS-6.4.3 (PHOTX)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)
1	1.20	1.19	1.19	**1.00**	**0.99**
7	2.74	2.77	2.72	**0.98**	**0.99**
10	4.83	4.99	4.78	**0.96**	**0.99**
20	41.8	48.5	43.2	**0.89**	**1.03**
30	393.	475.	418.	**0.88**	**1.06**

Table 3 Gamma-Ray Exposure Buildup Factors for Point Isotropic Source (1.0 MeV)

mfp	Water					Iron				
	EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)			EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)	A	B	C	(C/B)	(C/A)
1	2.10	2.08	2.06	**0.99**	0.98	1.86	1.85	1.85	**1.00**	**0.99**
7	15.9	15.8	15.5	**0.98**	0.97	10.1	10.0	10.1	1.01	1,00
10	26.4	26.1	25.6	**0.98**	0.97	16.0	15.8	15.9	1.01	0.99
20	74.3	74.0	72.4	**0.98**	0.97	41.0	41.3	41.7	1.01	1.02
30	138.	139.	136.	**0.98**	**0.99**	75.0	74.5	75.5	1.01	1.01

mfp	Lead				
	EGS4 (PHOTX)	ANS-6.4.3 (PHOTX)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)
1	1.38	1.38	1.36	**0.99**	**0.99**
7	2.95	2.89	2.86	**0.99**	**0.97**
10	3.62	3.51	3.46	**0.99**	**0.96**
20	5.45	5.27	5.12	**0.97**	**0.94**
30	7.10	6.64	6.49	**0.98**	**0.91**

Table 4 Gamma-Ray Exposure Buildup Factors for Point Isotropic Source (0.1 MeV)

mfp	Water					Iron				
	EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)			EGS4 (NBS)	ANS-6.4.3 (NBS)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)	A	B	C	(C/B)	(C/A)
1	4.68	4.55	4.32	**0.95**	**0.92**	1.39	1.40	1.37	**0.98**	**0.99**
7	148.	137.	130.	**0.95**	**0.88**	2.34	2.31	2.34	**1.01**	**1.00**
10	354.	321.	312.	**0.97**	**0.88**	2.66	2.61	2.68	**1.03**	**1.01**
20	2.35+3	2.17+3	2.30+3	**1.06**	**0.98**	3.43	3.33	3.62	**1.09**	**1.06**
30	8.56+3	7.97+3	9.21+3	**1.16**	**1.08**	4.02	3.86	4.47	**1.16**	**1.11**

mfp	Lead				
	EGS4 (PHOTX)	ANS-6.4.3 (PHOTX)	SN (JEF2)		
	A	B	C	(C/B)	(C/A)
1	2.17	2.04	2.11	**1.03**	**0.97**
7	43.2	54.9	43.6	**0.79**	**1.01**
10	243.	294.	251.	**0.85**	**1.03**
20	1.23+5	1.33+5	1.34+5	**1.01**	**1.09**
30	8.58+7	8.77+7	9.71+7	**1.11**	**1.13**

reported by Hirayama[9] and Kitsos et al.[8] are explained by the facts that bremsstrahlung sources are neglected in the moments calculations and the treatment of the bremsstrahlung in the PALLAS code includes some simplifications. In PALLAS, the multiple scattering of electrons is neglected and the bremsstrahlung radiation is emitted in the forward direction. These simplifications increase the photon flux, especially at deep penetrations. Table 2 gives the water, iron and lead exposure buildup factors at 10 MeV calculated without taking into account the secondary sources of bremsstrahlung. In this case the deviations observed between the different calculations are about 10%.

At 1 MeV where the Compton scattering effect is dominant (table 3), the buildup factors obtained by the different calculations are in very good agreement. The maximum deviations observed for all the materials are less than 10%.

At 0.1 MeV the lead buildup factors become very large at deep penetrations because of the K edge and the production of secondary sources of fluorescence. For this material, the maximum deviations observed between the Sn and EGS4 codes are about 10%. The deviations observed between the Sn and EGS4 codes on the one hand, and the standard data on the other hand, are about 20% at ~7mfp (table 4). For the water and the iron buildup factors, the different calculations are in good agreement. The deviations observed are about 10%.

2. Influence of coherent and Incoherent Scattering

Buildup factors found in literature[20,17,21,10] were calculated without taking into account coherent scattering when the Compton scattering was treated as a scattering on a free electron using the theory of Klein-Nishina. Hirayama and Trubey[22] evaluated the effect of neglecting coherent and incoherent scattering for water, iron, and lead up to 10 mfp; by using the Monte Carlo code EGS4. For incoherent scattering, the binding correction was taken into account only in the total cross section; the Klein-Nishina theory (without binding correction) was used for the differential cross section, a serious approximation. The results were reported in reference 10 as correction factors on the buildup factors. Subbaiah et al.[23] studied the influence of coherent scattering by using the ASFIT code; they originated the correction factors for coherent scattering used in reference 10. These correction factors concern only the coherent scattering, and their use causes difficulties because the effects of coherent and incoherent tend to cancel each other. It is better to either include or neglect both effects rather than to include

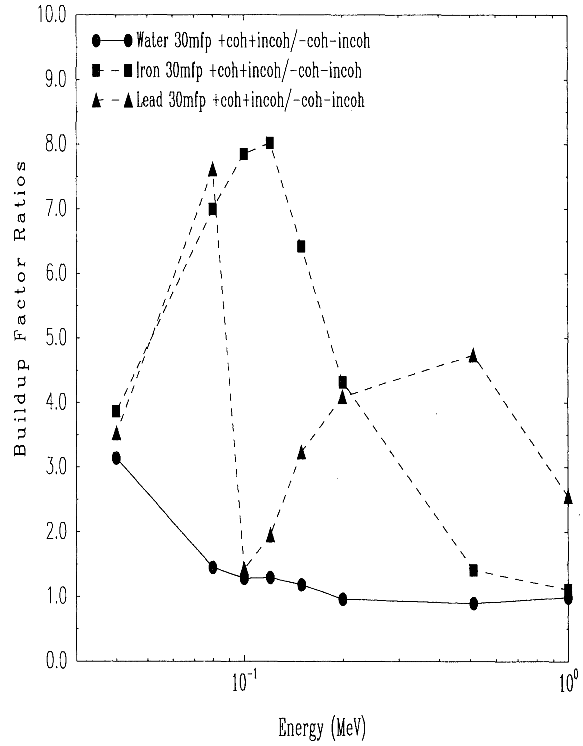

Fig. 1 Ratio of exposure buildup factors as a function of the energy source showing the influence of both the coherent and incoherent scattering, for water, iron and lead at 30 mean free paths.

or neglect only one of them in a transport calculations. Kitsos et al.[16] investigated in detail the influence of coherent and incoherent scattering on the exposures and the buildup factors by taking into account these effects in both the total and the differential cross sections; the secondary sources of fluorescence were neglected in their transport calculations.

Figure 1 shows the water, iron, and lead exposure buildup factors at 1 and 0.1 MeV, calculated with and without coherent and incoherent scattering.

At 1 MeV, the influence of the coherent and incoherent scattering is important only for lead; the both effects increase the buildup factors by a factor ~2.5 at 30 mfp.

At 0.1 MeV, the influence of coherent and incoherent scattering is important for all the materials; the water buildup factors are increased by about 30% at 30mfp, those of iron by a factor 8, and those for lead by about 50% above the K edge

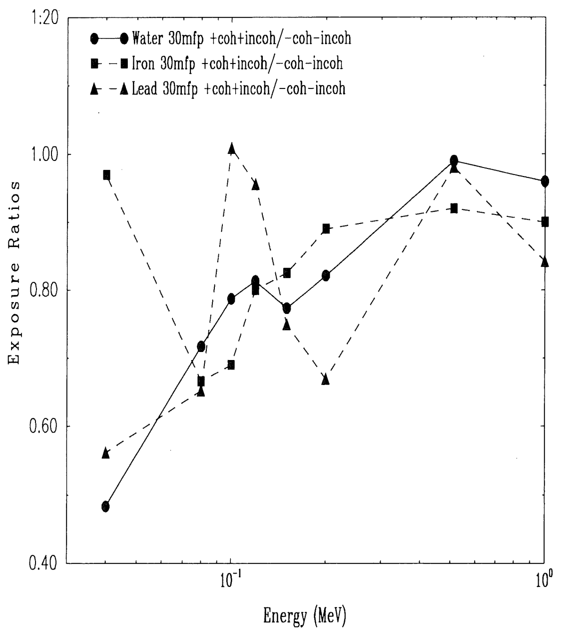

Fig. 2 Ratio of exposures as a function of the energy source for the same shielding thickness.

and about a factor 8 just below. The coherent and incoherent scattering are competitive with the photoelectric effect, which weakens their influence at low energies. Figure 1 shows that the iron and the lead buildup factors stop increasing and start to decrease when the photoelectric effect becomes preponderant.

Figure 2 shows the influence of both coherent and incoherent scattering on the exposures calculated at the same physical thickness. In this case, the exposure decreases if we take into account these effects because of an increase in the total cross section.

V. Conclusion

The aim of this paper was to compare point isotropic buildup factors recently calculated by Sn discrete ordinates codes with those obtained by Hirayama using the EGS4 code with a particle splitting technique and those of the standard data, ANS-6.4.3-1991. The comparisons were presented for the water, iron, and lead exposure buildup factors, for 3 typical energies of 10, 1, and 0.1 MeV, and for total thicknesses of up to 30 mfp. The comparisons have shown that the buildup factors calculated by the Sn and EGS4 codes are in very good agreement. The maximum deviations observed between the results given by these codes were about 10% for all cases. The deviations observed between the Sn and EGS4 codes on the one hand, and the standard data on the other hand, were about 35% for the iron and the lead exposure buildup factors at 10 MeV, and about 20% for the lead exposure buildup factors at 0.1 MeV.

In the second part of the study, we have shown the influence of both coherent and incoherent scattering on the buildup factors and the exposures. These effects are important for the energy range below 1 MeV and must not be neglected in the transport calculations.

The comparisons between the different calculations were carried out using different cross section compilations. This study could be completed by using the same g-ray cross section evaluation for all the transport codes.

Acknowledgments

The authors thanks Pr. Hirayama of the National Laboratory for High Energy Physics and Dr. Shin of the Kyoto University for their valuable discussions, suggestions, and communications.

— References —

(1) Harima, H. : *Radiat. Phys. Chem.*, **41**, 631 (1993).
(2) Dupont, C. : "MERCURE-5", *Internal Report*, Centre d'Études 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) Dejonghe, G., Luneville, L. : "SN1D", *Internal Report*, Centre d'Etudes de Saclay (1993).
(5) O'Dell, R. D., *et al.* : "ONEDANT", *LA*-9184, Los Alamos National Laboratory (1989).
(6) Nelson, W. R., Hirayama, H., Rogers, D. : "The EGS Code System", *SLAC*-265, Stanford Linear Accelerator Center, Stanford (1985).
(7) Takeuchi, K., Tanaka, S. : "PALLAS-1D(VII): A code for Direct Integration of Transport Equation in One Dimensional Plane and Spherical Geometries", *JAERI-M*84-214, (1984).
(8) Kitsos, S., *et al.* : *Nucl. Sci. Eng.*, **123**, 215(1996).
(9) Hirayama, H. : *J. Nucl. Sci. Technol.*, **32**, 1201(1995).
(10) Trubey, D. K. : "New Gamma-Ray Buildup Factor Data for Point Kernel Calculations: ANS-6.4.3 Standard Reference Data", *NUREG/CR*-5740, U.S. Nuclear Regulation Commission (1991).
(11) Files JEF-2, ENDF-B4, and ENDF-B6, OECD/NEA Data Bank, Nuclear Energy Agency (1991).
(12) Cullen, D. E., *et al.* : *UCRL*-50400, **Vol. 6**, Lawrence Livermore National Laboratory (1989).
(13) Hubbell, J., *et al.* : *J. Phys. Chem. Ref. Data*, **6**, 615(1977).
(14) Perkins, S. T., *et al.* : *UCRL*-50400, **Vol. 30**, Lawrence Livermore National Laboratory (1991).
(15) Assad, A. : *"PhD Thesis"*, University of Paris XI, Orsay (1995). (In French).
(16) Kitsos, S., *et al.* : *Nucl. Sci. Eng.*, **117**, 47(1994).
(17) Chilton, A. B., *et al.* : *Nucl. Sci. Eng.*, **73**, 97(1980).
(18) Hubbell, J. : *NSRDS-NBS*-29(1969).
(19) Radiation Shielding Information Center Data Package, *DLC*- 136/PHOTX, contributed by National Institute of Standards and Technology.
(20) Goldstein, H., Wilkins, J. E. : *NYO*-3075, Nuclear Development Associates (1954).
(21) Takeuchi, K., Tanaka, S. : *Nucl. Sci. Eng.*, **90**, 158(1985).
(22) Hirayama, H., Trubey, D. K. : *Nucl. Sci. Eng.*, **99**, 145(1988).
(23) Subbiah, K., *et al.* : *Nucl. Sci. Eng.*, **101**, 352(1989).