Original Article

Monte Carlo-based revised values of dose rate constants at discrete photon energies

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ABSTRACT

Absorbed dose rate to water at 0.2 cm and 1 cm due to a point isotropic photon source as a function of photon energy is calculated using the EDKnrc user-code of the EGSnrc Monte Carlo system. This code system utilized widely used XCOM photon cross-section dataset for the calculation of absorbed dose to water. Using the above dose rates, dose rate constants are calculated. Air-kerma strength S_k needed for deriving dose rate constant is based on the mass-energy absorption coefficient compilations of Hubbell and Seltzer published in the year 1995. A comparison of absorbed dose rates in water at the above distances to the published values reflects the differences in photon cross-section dataset in the low-energy region (difference is up to 2% in dose rate values at 1 cm in the energy range 30–50 keV and up to 4% at 0.2 cm at 30 keV). A maximum difference of about 8% is observed in the dose rate value at 0.2 cm at 1.75 MeV when compared to the published value. S_k calculations based on the compilation of Hubbell and Seltzer show a difference of up to 2.5% in the low-energy region (20–50 keV) when compared to the published values. The deviations observed in the values of dose rate and S_k affect the values of dose rate constants up to 3%.

Key words: Absorbed dose rate, air-kerma strength, brachytherapy, dose rate constant, TG-43

Introduction

Brachytherapy is one of the most popular modes of treatment due to its advantage of highly localized tumour dose delivery and at the same time sparing of normal tissues because of rapid dose fall off at various distances from the source. Dose rate constant Λ is one of the key parameters of the dose calculation protocol.[1,2] According to AAPM (American Association of Physicists in Medicine) Task Group (TG) 43 and TG43-U1,[1,2] the dose rate constant is defined as the dose rate to water at a distance of 1 cm on the transverse axis of a unit air-kerma strength source in a water phantom. This constant includes the effect of source geometry, the spatial distribution of radioactivity within the source, encapsulation and self-filtration within the source, and scattering in water surrounding the source. In case of intravascular brachytherapy, the distances of interest are much smaller than the conventional brachytherapy reference distance of 1 cm. According to AAPM TG-60,[3] the dose rate constant is defined as the dose rate at a reference distance of 2 mm in water from a source of unit air-kerma strength. Luxton and Gabor[4] calculated the absorbed dose rate to water as a function of distance from monoenergetic point photon sources in a unit density water phantom using the EGS4 Monte Carlo code system.[5] In their work, air-kerma strength S_k per unit photon from an isotropic point photon source is obtained as a function of energy using the mass-energy absorption coefficient of air published by Hubbell[6] in the year 1982. The revised data of mass-energy absorption coefficients were published by Hubbell and Seltzer[7] in the year 1995. Using the values of dose rate at 1 cm from the source in water phantom and S_k, Luxton and Gabor[4] calculated Λ as a function of photon energy. Chen and Nath[8] investigated the general properties of Λ and developed a simple analytical tool to calculate Λ. Selvam *et al.*[9] published the values of Λ from a point monoenergetic photon source as a function of photon energy (20 keV-1 MeV). The authors used Monte

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Carlo-based MCNP code (version 3.1)[10] which is not capable of transporting secondary electrons produced by the photons.

DeMarco *et al.*,[11] in their Monte Carlo study using the MCNP4C code,[12] emphasized that the photon cross-section dataset has to be updated to a modern tabulation such as DLC-146 or XCOM while simulating photons in the energy range 20-100 keV in materials of low atomic number such as water. Because, differences of up to 10% are observed in the photoelectric cross section for water at 30 keV between the standard MCNP cross-section dataset (DLC-200) and the most recent XCOM or NIST (National Institute of Standards and Technology) tabulation.

The aim of this work is to calculate the dose rate to water and Λ at 0.2 cm and 1 cm distances from an isotropic point photon source as a function of photon energy (20 keV-2 MeV) and compare the same with the published values. The Monte Carlo calculations are carried out using the EGSnrc code system[13,14] which utilizes the widely used XCOM photon cross-section dataset.[15] The study also includes comparison of published values of S_k by Luxton and Gabor[4] against the values based on mass-energy absorption coefficient of air by Hubbell and Seltzer.[7]

Materials and Methods

Calculation of S_k

According to TG-43U1[1,2] formalism, S_k is defined as air-kerma rate at the point along the transverse axis of the source in free space. In this study, the general formula proposed by Luxton and Gabor[4] is used to calculate S_k (μGy m²/h) as a function of energy E (keV) for a point source of activity A (MBq).

$$S_k(E) = C \times \frac{1}{4\pi} \times E \times A \times \left[\frac{\mu_{en}}{\rho}(E)\right]_{air} \quad .....(1)$$

where $\left[\frac{\mu_{en}}{\rho}(E)\right]_{air}$ is the mass-energy absorption coefficient (m²/kg) of air and C = 0.5768 μGy kg/h/keV/MBq. The point source is in vacuum, and therefore, exponential attenuation and scattering by air is not required.

Monte Carlo calculations

In the present study, point photon source is positioned at the center of the water sphere of diameter 1 m for energy below 500 keV and 1.3 m for energy of 500 keV and above. The dimensions of the water phantom considered are consistent with the approach adopted by Luxton and Gabor.[4] The absorbed dose rate per photon is scored in spherical shell of water of thickness 0.1 mm centered at distances of 0.2 cm and 1 cm from the point source. Density of water is taken as 0.998 g/cm³. The Monte Carlo-based user-code EDKnrc of the EGSnrc[14] code system is used for this purpose. The PEGS4 dataset needed for Monte Carlo calculations described above is based on XCOM[15] compilations. We set AE = 0.512 MeV (1 keV kinetic energy) and AP = 0.001 MeV while generating the PEGS4 dataset, where the parameters AE and AP are the low-energy thresholds for the production of knock-on electrons and secondary bremsstrahlung photons, respectively. All the calculations utilized the PRESTA-II step length and EXACT boundary crossing algorithms. In all calculations, electron range rejection technique is used to save computation time. We set ESAVE = 2 MeV for this purpose. The photon transport cut-off energy, PCUT, is chosen at 1 keV in all calculations. In EDKnrc calculations, we set AE = ECUT = 0.512 MeV (1 keV kinetic energy). We included bound Compton scattering and Rayleigh scattering in the calculations. Up to 10^8 photon histories

Table 1: Comparison of absorbed dose rate to water per disintegration at 1 cm times square of the distance (nGy cm²/h/Bq) due to a point isotropic photon source in liquid water

Photon energy (keV)	*Present study[a]*	*Luxton and Gabor[b]*	*Ratio* $= \frac{\text{Luxton \& Gabor}}{\text{present work}}$
20	0.3204	0.3204	1.000
30	0.2304	0.2265	0.983
40	0.1586	0.1556	0.981
50	0.1260	0.1236	0.981
60	0.1131	0.1121	0.991
70	0.1114	0.1101	0.988
80	0.1164	0.1157	0.994
90	0.1250	0.1243	0.994
100	0.1358	0.1347	0.992
125	0.1696	0.1674	0.987
150	0.2077	0.2060	0.992
175	0.2460	0.2445	0.994
200	0.2867	0.2861	0.998
250	0.3679	0.3640	0.989
300	0.4502	0.4447	0.988
350	0.5283	0.5283	1.000
400	0.6088	0.6033	0.991
500	0.7565	0.7602	1.005
600	0.8962	0.9056	1.010
700	1.0419	1.0342	0.993
800	1.1670	1.1651	0.998
900	1.2916	1.2805	0.991
1000	1.4093	1.4016	0.994
1170	1.6038	1.5977	0.996
1250	1.6871	1.6900	1.002
1330	1.7732	1.7823	1.005
1500	1.9481	1.9438	0.998
1750	2.1951	2.1630	0.985
2000	2.4272	2.4225	0.998

Depending on the photon energy, the values calculated in the present study have statistical uncertainties in the range of 0.1-0.4%, [a]Based on EDKnrc user-code of EGSnrc code system, [b]Luxton and Gabor[4] are simulated. Depending upon the photon energy, the 1σ statistical uncertainties on the calculated EDKnrc-based dose values are generally in the range 0.1-0.4%.

Calculation of Λ

Using the absorbed dose rate values at 1 cm and 0.2 cm from the point sources, dose rate constants at these distances are calculated as a function of photon energy E as below.

$$\Lambda(E)=\frac{\dot{D}(r_o=1\ cm)}{S_k} \quad .....(2)$$

where $\dot{D}(r_o=1cm)$ is the absorbed dose rate to water (cGy/h) at $r_0 = 1$ cm from the point source.

$$\Lambda(E)=\frac{\dot{D}(r_o=0.2\ cm)}{S_k} \quad .....(3)$$

where $\dot{D}(r_o=0.2cm)$ is the absorbed dose rate to water (cGy/h) at $r_0 = 0.2$ cm from the point source.

Results and Discussion

Dose rate

Table 1 compares the values of absorbed dose rate to water per disintegration at 1 cm from the source times square of the distance from the source (nGy cm^2/h/Bq) calculated using the EDKnrc and those published by Luxton and Gabor.[4] The comparison shows that the values calculated in the present study are higher by about 2% than the published values in the energy range 30-50 keV. This difference is due to the most recent XCOM/NIST cross-section dataset used in the EDKnrc-based calculations. In the rest of energy region, the agreement is within 0.5%.

Table 2 compares the values of absorbed dose rate to water per disintegration at 0.2 cm from the source times square of the distance from the source (nGy cm^2/h/Bq) calculated using the EDKnrc and those published by Luxton and Gabor[4] and Selvam *et al.*[9] The comparison (see column 5) against the values published by Selvam *et al.*[9] shows about

Table 2: Comparison of absorbed dose rate to water per disintegration at 0.2 cm times square of the distance (nGy cm^2/h/Bq) due to a point isotropic photon source in liquid water

Photon energy (keV)	*Present work*[a]	*Selvam et al.*[b]	*Luxton and Gabor*[c]	$Ratio=\frac{Selvam\ et\ al.}{present\ work}$	$Ratio=\frac{Luxton\ \&\ Gabor}{present\ work}$
20	0.4775	0.4827	0.4674	1.011	0.979
30	0.2257	0.2238	0.2170	0.992	0.961
40	0.1368	0.1359	0.1361	0.993	0.995
50	0.1047	0.1034	0.1016	0.987	0.970
60	0.0944	0.0930	0.0923	0.985	0.978
70	0.0939	-	0.0941	-	1.002
80	0.1000	0.0995	0.0990	0.995	0.990
90	0.1095	-	0.1108	-	1.012
100	0.1207	0.1204	0.1226	0.998	1.016
125	0.1549	-	0.1519	-	0.981
150	0.1937	0.1932	0.1952	0.997	1.008
175	0.2347	-	0.2343	-	0.998
200	0.2764	0.2749	0.2736	0.994	0.990
250	0.3602	-	0.3570	-	0.991
300	0.4434	0.4405	0.4455	0.993	1.005
350	0.5255	-	0.5281	-	1.005
400	0.6054	0.6016	0.6075	0.994	1.003
500	0.7624	0.7555	0.7730	0.991	1.014
600	0.9177	0.9012	0.9211	0.982	1.004
700	1.0706	-	1.0678	-	0.997
800	1.2258	1.1719	1.1947	0.956	0.975
900	1.3283	-	1.3473	-	1.014
1000	1.3604	1.4184	1.3511	1.043	0.993
1170	1.3115	-	1.3327	-	1.016
1250	1.2719	-	1.3158	-	1.034
1330	1.2380	-	1.2845	-	1.038
1500	1.1544	-	1.2067	-	1.045
1750	1.0520	-	1.1324	-	1.076
2000	0.9679	-	0.9795	-	1.012

Depending on the photon energy, the values calculated in the present study have statistical uncertainties in the range of 0.1–0.4%. The dose rate values reported by Selvam *et al.*[9] have uncertainties in the range of 0.04-0.07%, [a]Based on EDKnrc user-code of EGSnrc code system, [b]Selvam *et al.*[9], [c]Luxton and Gabor[4]

4% difference at high energies (800 and 1000 keV). This is due to the fact that MCNP (version 3.1)[10] calculations did not include detailed electron transport and, therefore, collision kerma was approximated to the absorbed dose. Auxiliary simulations by setting ECUT = 2 MeV in the EDKnrc user-code produced comparable dose rate values at photon energies E = 600, 800, and 1000 keV against the values reported by Selvam *et al.*[9] Note that calculation using ECUT = 2 MeV in the EDKnrc user-code is equivalent to scoring water-kerma, as the secondary electrons will deposit their energy where they are generated. The last column of Table 2 shows the comparison of dose rate values calculated in the present study and those by Luxton and Gabor.[4] The differences are significant at both low-energy and high-energy regions. In the low-energy region, the difference is up to 4% (at 30 keV). In the high-energy region, the difference is between 2% and 8% (8% at 1750 keV). At 2 MeV, the comparison is within about 1%.

Air-kerma strength

Table 3 compares the values of S_k calculated in the present study against the values published by Luxton and Gabor.[4] In lower energy range (up to 60 keV), the variation in the S_k is about 2%. This difference is because the calculation of S_k by Luxton and Gabor[4] was based on mass-energy absorption coefficient of air published by Hubbell[6] in 1982, whereas the present study utilized the mass-energy absorption coefficient of air published by Hubbell and Seltzer[7] in 1995.

Table 3: Comparison of air-kerma strength S_k per Bq (nGy cm^2/h/Bq) (1 Bq=1 photon/s)

Photon energy (keV)	Present work[a]	Luxton and Gabor[b]	Ratio = $\frac{\text{Luxton \& Gabor}}{\text{present work}}$
20	0.4945	0.4829	0.977
30	0.2116	0.2065	0.976
40	0.1254	0.1228	0.979
50	0.0940	0.0925	0.984
60	0.0837	0.0827	0.988
80	0.0884	0.0879	0.994
100	0.1067	0.1064	0.997
150	0.1718	0.1717	0.999
200	0.2452	0.2453	1.000
300	0.3953	0.3952	0.999
400	0.5412	0.5414	1.000
500	0.6804	0.6807	1.000
600	0.8129	0.8132	1.000
800	1.0579	1.0583	1.000
1000	1.2796	1.2792	0.999
1250	1.5313	1.5296	0.999
1500	1.7550	1.7522	0.998
2000	2.1519	2.1499	0.999

[a]Based on Hubbell and Seltzer[7], [b]Luxton and Gabor values based on Hubbell[6]

Dose rate constant

Note that the differences in the values of absorbed dose to water and S_k as discussed above will directly affect the value of Λ. Table 4 compares the values of Λ in the present work against the values published by Luxton and Gabor[4] and Chen and Nath.[8] Λ is based on dose rate to water at 1 cm from a point isotropic photon source. The values reported by Luxton and Gabor[4] show agreement at all energies except at 20 keV where the overestimation is 2.4%. This is because the dose rate values at 1 cm and S_k obtained in the present study are higher by 2% in the energy range 30-50 keV when compared to the corresponding values reported by Luxton and Gabor.[4] Hence, there is no variation in the Λ values. Whereas at 20 keV, the dose rates at 1 cm compare well [Table 1], and hence, a difference of about 2% in the Λ value is observed.

The analytical calculation of Λ by Chen and Nath[8] utilized the Monte Carlo-based energy absorption buildup factors reported by Angeloupos *et al.*[16] These buildup factors may not be accurate in the low-energy region as the calculations were based on old cross-section dataset. Hence, the values of Λ calculated in the present study are higher in the lower energy region (higher by about 3% at 50 and 60 keV).

Table 5 compares the values of Λ in the present work against those published by Selvam *et al.*[9] and Luxton and Gabor.[4] Λ is based on dose rate to water at 0.2 cm from a point isotropic photon source. The differences in the values reflect the differences observed in the dose rate values, as the present study and the work by Selvam *et al.*[9] utilized the same mass-energy absorption coefficient of air.[7] Differences shown in the last column of the Table 5 (present work vs. Luxton and Gabor[4]) reflect the combined effect of differences observed in the dose rate values [Table 2] and the different dataset used for calculating S_k. Dose rate calculations using ECUT = 2 MeV in the EDKnrc produced Λ values of 27.64, 27.81, and 27.73 cGy cm^2/h at photon energies E = 600, 800, and 1000 keV, respectively, which compare well with the corresponding values reported by Selvam *et al*.[9]

Conclusion

EDKnrc-based calculations show that dose rate values in water at 1 cm from the point photon sources are higher by about 2% than the published values in the energy range 30-50 keV. This difference is attributed to the most recent XCOM/NIST cross-section dataset used in the EDKnrc calculations. Regarding dose rate values at 0.2 cm from the source, the differences are significant at both low-energy and high-energy regions when compared to the published values. In the low-energy region, the difference is up to 4% (at 30 keV) and at 1.75 MeV, the difference is about 8%. The study suggests that the recent compilation of mass-energy absorption

Table 4: Comparison of dose rate constant Λ (cGy/h/U)

Photon energy (keV)	*Present work*	*Luxton and Gabor*[a]	*Chen and Nath*[b]	$Ratio = \frac{Luxton\,\&\,Gabor}{present\ work}$	$Ratio = \frac{Chen\,\&\,Nath}{present\ work}$
20	0.6480	0.6635	0.6490	1.024	1.002
30	1.0892	1.0965	1.0860	1.007	0.997
40	1.2650	1.2666	1.2500	1.001	0.988
50	1.3398	1.3357	1.3000	0.997	0.970
60	1.3515	1.3552	1.3120	1.003	0.971
80	1.3178	1.3165	1.2940	0.999	0.982
100	1.2726	1.2658	1.2590	0.995	0.989
150	1.2090	1.1999	1.1930	0.992	0.987
200	1.1692	1.1663	1.1590	0.998	0.991
300	1.1389	1.1253	1.1330	0.988	0.995
400	1.1248	1.1143	1.1220	0.991	0.998
500	1.1118	1.1168	1.1140	1.004	1.002
600	1.1024	1.1135	1.1070	1.010	1.004
800	1.1032	1.1010	1.0970	0.998	0.994
1000	1.1013	1.0957	1.0940	0.995	0.993
1250	1.1018	1.1049	-	1.003	-
1500	1.1100	1.1093	-	0.999	-
2000	1.1280	1.1268	-	0.999	-

Λ is based on dose rate to water at 1 cm from a point isotropic photon source. Depending on the photon energy, the values calculated in the present study have statistical uncertainties in the range of 0.1-0.4%, [a]Luxton and Gabor[4], [b]Chen and Nath[8]

Table 5: Comparison of dose rate constant Λ (cGy/h/U)

Photon energy (keV)	*Present work*	*Selvam et al.*[a]	*Luxton and Gabor*[b]	$Ratio = \frac{Selvam\ et\ al.}{present\ work}$	$Ratio = \frac{Luxton\,\&\,Gabor}{present\ work}$
20	24.1386	24.401	24.1976	1.011	1.002
30	26.6697	26.451	26.2712	0.992	0.985
40	27.2641	27.086	27.7077	0.993	1.016
50	27.8433	27.488	27.4595	0.987	0.986
60	28.1766	27.786	27.9021	0.986	0.990
80	28.2927	28.159	28.157	0.995	0.995
100	28.2866	28.228	28.8064	0.998	1.018
150	28.1849	28.115	28.4217	0.997	1.008
200	28.1857	28.027	27.8842	0.994	0.989
300	28.0410	27.857	28.1819	0.993	1.005
400	27.9627	27.788	28.0523	0.994	1.003
500	28.0116	27.757	28.3899	0.991	1.014
600	28.2213	27.715	28.3171	0.982	1.003
800	28.9698	27.695	28.2221	0.956	0.974
1000	26.5785	27.710	26.4052	1.043	0.993

Λ is based on dose rate to water at 0.2 cm from a point isotropic photon source. Depending on the photon energy, the values calculated in the present study have statistical uncertainties in the range of 0.1-0.4%. Λ values reported by Selvam *et al*.[9] have uncertainties in the range of 0.04-0.07%, [a]Selvam *et al*.[9], [b]Luxton and Gabor[4]

coefficient of air by Hubbell and Seltzer[7] is important for air-kerma strength calculations, as a difference of up to 2.5% is observed in the low-energy photons (20-50 keV). The deviations observed in the values of dose rate and air-kerma strength affect dose rate constants up to 3%.

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