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論 文

Derivation of a Monte Carlo Estimator for Dose Equivalent

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=**Abstract**=

An alternative estimator for dose equivalent was derived. The original LET distribution concept was transformed into a charged particle fluence spectrum concept along with the definition of an average quality factor named *slowing-down averaged quality factor* by adopting the continuous slowing down approximation. With the alternative estimator, the dose equivalent delivered into a receptor located in a given radiation field can be directly and conveniently estimated in a Monte Carlo procedure. The slowing-down averaged quality factors for the energy range below 10 MeV were evaluated and tabulated for the charged particles which may be generated from the interactions of neutron with the nuclei composing soft tissue.

1. Introduction

The dose equivalent is a quantity to be used in the radiation protection field as a measure of the deleterious effect of radiation on health. Currently this radiation quantity is defined by modifying the absorbed dose by a dimensionless quantity called quality factor which is adopted to take into account the different health effects of radiations having different qualities;

$$H=\int_0^\infty Q(L_\infty)D(L_\infty)dL_\infty \qquad (1)$$

where H is the dose equivalent, $Q(L_\infty)$ is the quality factor given as a function of the unrestricted linear energy transfer (LET or stopping power) L_∞ and $D(L_\infty)$ is the LET distribution of absorbed dose[1].

The relationship between LET in water and quality factor is specified by the International Commission on Radiological Protection (ICRP)[2]. Since photons and electrons have low LET values, the quality factors for these particles are assigned to 1.0. Therefore evaluation of Eqn. (1) for photons and electrons is straightforward. For neutrons, on the other hand, the evaluation is much more complicated because several kinds of charged particles are generated from the interactions of neutrons with the nuclei in tissue and the LET values of the charged particles vary significantly as the particles slow down in the midium.

Jones *et al*[3]. estimated dose equivalents by the Monte Carlo method using the original concept in which the LET distributions of absorbed dose were constructed and numerically integrated. However, the construction of the LET distribution in a Monte Carlo procedure must be a tedious task. Similarly

Zerby and Kinney[4] used a transformed estimator to construct rough energy distributions of absorbed dose and to compute the dose equivalent by use of average values of quality factor.

Cross and Ing[5] calculated mean quality factors as a function of neutron energy by weighting the kerma in tissue for charged particles produced from the neutron interactions. The resulting mean quality factor, along with the kerma factor, can be used in the computation of dose equivalent by combining with any known neutron fluence spectrum in a medium. The fluence spectrum in the receptor may be provided by an independent Monte Carlo calculation. This approach, i.e., a separate calculation of neutron spectra and quality factors, has some advantages; the statistical errors resulting from the Monte Carlo estimation can be reduced and the same quality factors can be applied to calculated spectra in different receptors. However this estimation method cannot accommodate particle escape effect at the surface layer of the receptor since the point detector concept (or first collision concept) is employed through the kerma approximation of absorbed dose.

In order to overcome the tediousness in the construction of the LET distribution of absorbed dose for the direct estimation of the dose equivalent in a Monte Carlo procedure, an alternative estimator is derived in this study. The derivation is given in the next section and the slowing-down averaged quality factors, which are required for the alternative estimation, are provided for the charged particles which may be generated from the interactions of neutrons with soft tissue prescribed by the International Commission on Radiation Units and Measurements (ICRU)[6].

2. Derivation of the Alternative Dose Equivalent Estimator

By transforming the independent variable in Eqn. (1), one can get

$$H=\int_0^{E_m} Q(E)D(E)\,dE \tag{2}$$

where E is the energy of the charged particle and E_m is the maximum energy the charged particle can have. Assume a unit volume of absorber situated in a radiation field of charged particles and let the fluence per unit energy be $\Phi(E)$. Then the absorbed dose resulted from the charged particles having energies between E and $E+dE$, $D(E)dE$, is

$$D(E)\,dE=\frac{\Phi(E)\,dE\cdot L_\infty(E)}{\rho} \tag{3}$$

where ρ is the density of the medium.

Under the continuous slowing down approximation (CSDA), all particles having energies greater than E should slow down through the energy interval $(E, E+dE)$. If we assume that the CSDA is valid for dosimetric purpose, the differential fluence in dE about E becomes

$$\Phi(E)\,dE=\frac{N\,dx}{V}$$

where V is the detector volume, dx is the track length created by the particle during slowing down from $E+dE$ to E and N is the total number of charged particles whose energies are greater than E, i.e.,

$$N(E)=\int_E^\infty n(E_0)\,dE_0$$

Here the term $n(E_0)dE_0$ is the number of charged particles in the energy interval (E_0, E_0+dE_0) or the fluence spectrum.

Recall the definition of the linear energy transfer, that is $L_\infty=dE/dx$, to get

$$\Phi(E)\,dE=\frac{dE}{VL_\infty(E)}\int_E^{E_m} n(E_0)\,dE_0 \tag{4}$$

Substitution of Eqn. (4) into Eqn. (3) yields

Table 1. Recommended values of quality factor and the calculated spline coefficients

Linear energy transfer[a], L_i (keV/μm)	Quality factor[b], Q_i	Cubic spline coefficients[c]			
		a_{0j}	a_{1j}	a_{2j}	a_{3j}
3.5	1.0				
		1.0	1.66608	−0.612982	0.419390
7.0	2.0				
		2.0	1.42080	0.259114	0.560274
23.0	5.0				
		5.0	4.41583	2.258590	−0.447446
53.0	10.0				
		10.0	7.25130	1.138010	−0.167440
175.0	20.0				

(a) Linear energy transfer in water(unrestricted).
(b) Recommended by the ICRP.
(c) Used in the interpolation formula;
$Q(L)=a_{0j}+D(a_{1j}+D(a_{2j}+a_{3j}D))$, $L_i \leq L < L_{i+1}$
where $D=\log L-\log L_i$.

$$D(E)\,dE=\frac{dE}{m}\int_{E}^{Em} n(E_0)\,dE_0 \qquad (5)$$

where m is the mass of the detector. Note that Eqn. (5) can be directly deduced from the concept of the absorbed dose. Equations (2) and (5) give

$$H=\frac{1}{m}\int_0^{Em} Q(E)\,dE\int_E^{Em} n(E_0)\,dE_0 \qquad (6)$$

By changing the order of integration in Eqn. (6), we get

$$H=\frac{1}{m}\int_0^{Em} n(E_0)\,dE_0\int_0^{E_0} Q(E)\,dE$$

or

$$H=\frac{1}{m}\int_0^{Em} dE_0 n(E_0)\,E_0\bar{Q}_{sl}(E_0) \qquad (7)$$

where the term $\bar{Q}_{sl}(E_0)$ is defined by

$$\bar{Q}_{sl}(E_0)\equiv\frac{1}{E_0}\int_0^{E_0} Q(E)\,dE \qquad (8)$$

and named *slowing-down averaged quality factor.**

In order to estimate the dose equivalent using Eqn. (1) in the Monte Carlo calculation, the LET distribution of absorbed dose has to be constructed first and then the integration is carried out by a numerical method. It is obviously a tedious task. Also many computer storages are needed to store the distribution data. Equation (7) can be used directly, on the other hand, in the estimation of the dose equivalent;

$$H=\frac{C}{m}\sum_i E_i\omega_i\bar{Q}_{sl}(E_i) \qquad (9)$$

where C is the conversion fator having value of 1.131×10^{-13}Gy−g/eV and ω is the statistical weight of the parent particle which generates the charged particle whose contribution to the dose equivalent is being estimated.

* The term "slowing-down averaged" is used since Eqn. (8) represents the mean value of the quality factor for monoenergetic charged particles of initial energy E_0 while slowing down to zero energy. A simple term such as "mean" may cause difficulty in identifying it from the term "average" or "effective" which is termed for different quantity by the ICRU and ICRP.

3. Calculation of the Slowing-down Averaged Quality Factors

For the calculation of the slowing-down averaged quality factor defined by the Eqn. (8), the quality factor values recommended by the ICRP as a function of the linear energy transfer in water were represented by cubic equations of $\log L$ using the cubic spline interpolation scheme[7].

$$Q(L)=\sum_{j=0}^{3} a_{ij}(\log L-\log L_i)^j,$$
$$L_i\leq L\leq L_{i+1} \qquad (10)$$

Table 2. Slowing-down averaged quality factors

INITIAL ENERGY (EV)[a]	CHARGED PARTICLES										
	H-1	O-16	C-12	N-14	H-2	H-3	HE-4	BE-9	C-13	C-14	B-11
1.0000E+07	3.14	20.00	20.00	20.00	4.50	5.53	14.92	19.99	20.00	20.00	20.00
6.3096E+06	3.98	20.00	20.00	20.00	5.65	6.90	16.95	19.99	20.00	20.00	29.99
3.9811E+06	5.05	20.00	20.00	20.00	7.08	8.49	18.56	19.98	20.00	20.00	20.00
2.5119E+06	6.36	20.00	20.00	20.00	8.69	10.12	19.58	19.97	20.00	20.00	19.99
1.5849E+06	7.89	20.00	20.00	20.00	10.30	11.56	19.80	19.95	20.00	20.00	19.99
1.0000E+06	9.53	20.00	20.00	20.00	11.72	12.67	19.65	19.92	20.00	20.00	19.99
6.3096E+05	11.06	20.00	20.00	20.00	12.77	13.32	19.45	19.87	20.00	20.00	19.98
3.9811E+05	12.31	20.00	19.99	20.00	13.36	13.48	19.14	19.79	19.99	20.00	19.96
2.5119E+05	13.13	20.00	19.99	19.99	13.46	13.17	18.61	19.66	19.99	19.99	19.94
1.5849E+05	13.46	19.99	19.99	19.99	13.09	12.45	17.84	19.47	19.99	19.99	19.91
1.0000E+05	13.31	19.99	19.98	19.99	12.33	11.43	16.49	19.15	19.98	19.98	19.85
6.3096E+04	12.73	19.98	19.97	19.98	11.28	10.24	14.87	18.66	19.97	19.97	19.76
3.9811E+04	11.80	19.98	19.95	19.97	10.06	8.97	13.40	17.93	19.95	19.95	19.94
2.5119E+04	10.63	19.96	19.91	19.95	8.78	7.77	12.16	17.29	19.92	19.93	19.40
1.5849E+04	9.35	19.94	19.86	19.92	7.57	6.74	11.15	16.89	19.87	19.88	19.14
1.0000E+04	8.05	19.90	19.78	19.87	6.54	5.94	10.38	16.64	19.80	19.81	18.91
6.3096E+03	6.89	19.85	19.66	19.80	5.73	5.35	9.85	16.45	19.68	19.70	18.66
3.9811E+03	5.92	19.76	19.46	19.67	5.12	4.96	9.50	16.22	19.49	19.53	18.34
2.5119E+03	5.14	19.62	19.14	19.49	4.70	4.73	9.28	15.92	19.20	19.25	17.91
1.5849E+03	4.36	19.40	18.63	19.18	4.42	4.62	9.12	15.51	18.73	18.82	17.36
1.0000E+03	4.13	19.03	17.88	18.71	4.26	4.58	8.94	14.98	18.00	18.10	16.68
6.3096E+02	3.83	18.49	16.98	17.93	4.16	4.57	8.72	14.33	17.08	17.18	15.89
3.9811E+02	3.61	17.57	15.98	16.87	4.09	4.55	8.41	13.57	16.08	16.16	14.66
2.5119E+02	3.45	16.36	14.90	15.71	4.01	4.49	8.03	12.72	14.99	15.06	14.00
1.5849E+02	3.30	15.07	13.76	14.49	3.91	4.38	7.57	11.79	13.84	13.90	12.95
1.0000E+02	3.16	13.76	12.58	13.23	3.78	4.21	7.05	10.81	12.64	12.69	11.85
6.3096E+01	3.01	12.43	11.37	11.96	3.61	4.00	6.47	9.79	11.43	11.47	10.72
3.9811E+01	2.85	11.10	10.17	10.69	3.41	3.75	5.87	8.76	10.21	10.25	9.58
2.5119E+01	2.68	9.81	8.98	9.44	3.18	3.48	5.26	7.75	9.02	9.05	8.46
1.5849E+01	2.50	8.56	7.84	8.23	2.95	3.20	4.67	6.76	7.87	7.89	7.38
1.0000E+01	2.31	7.38	6.75	7.10	2.71	2.91	4.12	5.84	6.78	6.80	6.37
6.3096E+00	2.12	6.29	5.76	6.05	2.47	2.64	3.61	5.00	5.78	5.80	5.44
3.9811E+00	1.93	5.31	4.88	5.11	2.23	2.38	3.16	4.26	4.89	4.90	4.61
2.5119E+00	1.74	4.46	4.12	4.30	2.01	2.13	2.77	3.63	4.13	4.13	3.90
1.5849E+00	1.56	3.75	3.48	3.63	1.79	1.90	2.42	3.10	3.49	3.49	3.31
1.0000E+00	1.38	3.16	2.95	3.07	1.59	1.68	2.12	2.66	2.96	2.96	2.82
6.3096E-01	1.21	2.68	2.52	2.61	1.39	1.47	1.85	2.29	2.53	2.53	2.42
3.9811E-01	1.07	2.29	2.16	2.23	1.22	1.28	1.61	1.97	2.17	2.17	2.08
2.5119E-01	1.01	1.96	1.86	1.92	1.07	1.12	1.38	1.70	1.86	1.86	1.79
1.5849E-01	1.00	1.68	1.59	1.64	1.00	1.02	1.19	1.45	1.59	1.60	1.53
1.0000E-01	1.00	1.43	1.36	1.40	1.00	1.00	1.04	1.24	1.36	1.36	1.31
6.3096E-02	1.00	1.22	1.16	1.20	1.00	1.00	1.00	1.07	1.17	1.17	1.12
3.9811E-02	1.00	1.05	1.03	1.04	1.00	1.00	1.00	1.00	1.03	1.03	1.02
2.5119E-02	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
1.5849E-02	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
1.0000E-02	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

(a) The initial energies of charged particles are given in equal logarithmic energy interval.

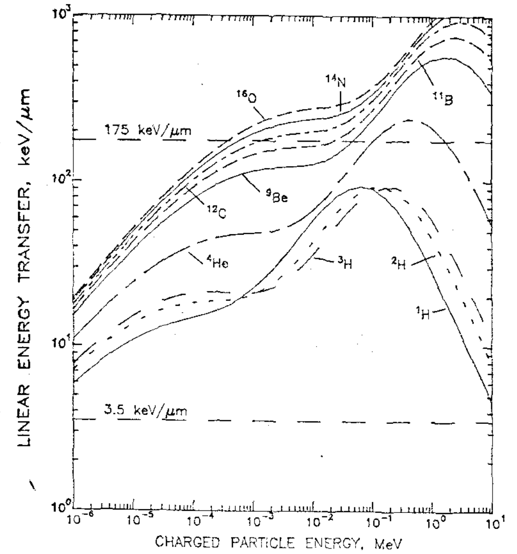

Fig. 1. Unrestricted linear energy transfer of charged particles in water (Calculated with the SPAR code).

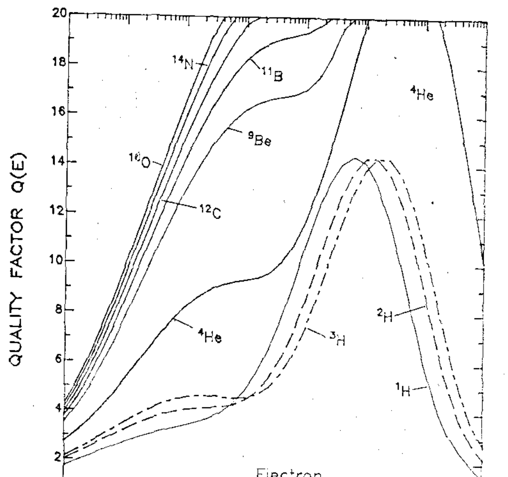

Fig. 2. Quality factors of charged particles as a function of their energies.

where a_{ij}'s are the spline coefficients, L_i is the linear energy transfer shown in Table 1 and the subscript ∞ which denotes the infinite cut-off energy in the representation of the LET is omitted for simplicity. The recommended values of Q and the spline coefficients calculated are tabulated in Table 1.

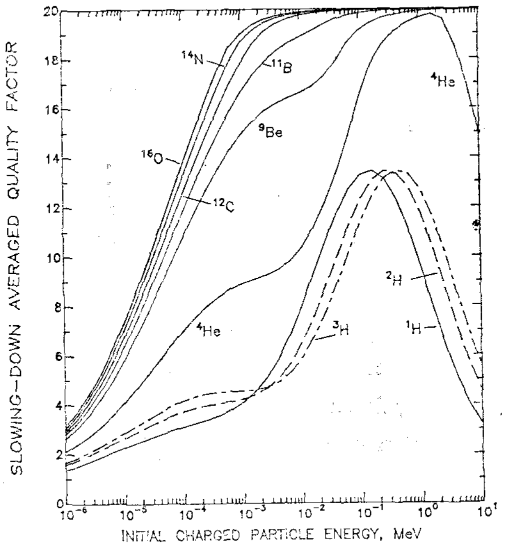

Fig. 3. Slowing-down averaged quality factors as a function of the initial energy of the charged particles.

If the linear energy transfer is known for a given value of charged particle energy, the corresponding quality factor can be determined with Eqn. (10). By repeating these calculations, one can get E_0-Q tables for each charged particle type. In the calculation, the LET in water was computed with the computer code SPAR[8] which was developed to calculate the stopping powers in any given medium. Some modifications of the SPAR code were made for the evaluation of Eqn. (10) with the stopping powers calculated. Figures 1 and 2 show the unrestricted linear energy transfer values in water and the quality factors, respectively, as a function of the charged particle energy for the types of charged particles which can be generated from the neutron-tissue interaction.

Since $Q(E)$ is a smooth function of the charged particle energy E as shown in Fig. 2, application of the cubic spline scheme in the E-$Q(E)$ relationship gives

$$Q(E)=\sum_{j=0}^{3}b_{ij}(E-E_i)^j,\quad E_i\leq E<E_{i+1}$$

where E_i's are the tabulated energy points and b_{ij}'s are the spline coefficients. Then Eqn. (8) can be written by

$$\bar{Q}_{st}(E_0)=\frac{1}{E_0}\left\{\sum_{k=1}^{i-1}\left(\frac{b_{k3}}{4}\delta_k^4+\frac{b_{k2}}{3}\delta_k^3+\frac{b_{k1}}{2}\delta_k^2+b_{k0}\delta_k\right)+\frac{b_{i3}}{4}\delta^4+\frac{b_{i2}}{3}\delta^3+\frac{b_{i1}}{2}\delta^2+b_{i0}\delta\right\} \tag{11}$$

where $\delta_k=E_{k+1}-E_k$ and $\delta=E_0-E_i$. Adoption of this procedure in the SPAR code gives the slowing-down averaged quality factor $\bar{Q}_{st}$ as a function of the initial energy of a given charged particle. The calculated values of $\bar{Q}_{st}$ are plotted in Fig. 3 and are given in Table 2 for future applications.

4. Conclusions

A dose equivalent estimator utilizing the charged particle fluence spectrum and the slowing-down averaged quality factor was derived to be adopted in the Monte Carlo dosimetric calculations. The continuous slowing down approximation was assumed in the derivation. The new estimator can be evaluated at each interaction site in the receptor provided that the type and energy of the secondary charged particles are determined. Therefore the contruction of the LET or energy distributions of absorbed dose is not needed.

Another advantage of the estimation method proposed in this study is that the computer memories needed to store the LET or energy distribution data can be saved. For such a problem as a depth-dose determination where number of detectors are defined, this saving will be valuable.

The slowing-down averaged quality factors which should be known for application of the new estimator were computed by means of a modified version of the SPAR code. The tabulated values of the slowing-down averaged quality factors for the charged particles generated from the intractions of neutrons having energies up to 10 MeV with soft tissue can be used in any dosimetric calculations in that energy range.

An extension of this work for higher energy particles would be interesting when more knowledge and better modeling of the nuclear interaction mechanism for high energy particles are achieved.

REFERENCES

1) International Commission on Radiation Units and Measurements, "Radiation quantities and units", ICRU Report 33(1980).
2) International Commission on Radiological Protection, "Data for protection against ionizing radiation from external sources: Supplement to ICRP publication 15", ICRP publication 21, Pergamon press, New York(1983).
3) T.D. Jones, W.S. Synder and J.A. Auxier, "Absorbed dose, dose equivalent and LET distributions in cylindrical phantoms irradiated by a collimated beam of monoenergetic neutrons", *Health Phys.*, **21**, 253-272 (1971).
4) C.D. Zerby and W.E. Kinney, "Calculated tissue current-to-dose conversion factors for nucleons below 400 MeV", *Nucl. Inst. and Methods*, **36**, 125-140(1965).
5) W.G. Cross and H. Ing, "Quality factors for monoenergetic neutrons", *Radiat. Res.*, **99**, 1-19(1984).
6) International Commission on Radiation Units and Measurements, "Radiation quantities and units", ICRU Report 19(1971).
7) G.E. Forsythe, M.A. Malcolm, *et al.*, Computer Methods for Mathematical Computations, Prentice Hall(1977).
8) T.W. Armstrong and K.G. Chandler, "SPAR,

a FORTRAN program for computing stopping powers and ranges for muons, charged pions, protons and heavy ions", Oak Ridge National Laboratory report, ORNL-4869(1974).

몬테칼로법을 위한 선량당량 산정법의 도출

이 재 기

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=요 약=

연속감속근사법(CSDA)과 감속평균선질계수를 이용하여 선량당량 정의에서의 본래의 LET 분포 개념을 하전입자속 스펙트럼의 개념으로 변환함으로써 새로운 선량당량 산정법을 도출하였다. 이 산정법을 몬테칼로법에 적용함으로써 주어진 방사선장에 위치한 피사체 내에서의 선량당량을 직접적으로 간편하게 산출할 수 있다. 산정에 필요한 감속평균 선질계수는 중성자와 연조직과의 상호작용으로부터 발생될 수 있는 모든 하전입자에 대하여 10 MeV 이하의 에너지 범위에서 산출하여 제시하였다.