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Calculation of Local Energy Deposition Due to Electron Capture and Internal Conversion

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Absorbed dose calculations for internally administered radionuclides require the determination of E_β, "the total local energy deposition per disintegration". Most of the absorbed dose from β- and γ-emitting radionuclides is, with exceptions such as ^{60}Co and ^{22}Na, due to β particles and conversion electrons. The quantity, $\bar{E}_\beta$, however, is really defined only for β particles, *i.e.* electrons originating in the nucleus. To this quantity must be added the energy of all electrons appearing in decay processes as well as photons whose ranges are comparable to electron ranges.

Recently, there has been an increase in the use of radionuclides which decay primarily by electron capture. For some of these, there are no readily available values of the total "beta-type" energy released, E_β, as distinguished from $\bar{E}_\beta$, the average energy of emitted beta particles only. Although the radionuclides that decay by electron capture may not emit beta particles, they may contribute substantially to an on-site absorbed dose by conversion and Auger electrons and by relatively large amounts of low energy x-rays.

Previously calculated and experimentally determined values of the total "beta-type" energy release appear to have been sufficiently accurate for most radionuclides. (This quantity has been designated by E, $\bar{E}$, $[E_\beta]$, or another symbol to distinguish it from the average energy of emitted beta particles only.) Recently, however, there has been an increase in the use of some radionuclides of exceptional interest in nuclear medicine which decay primarily by electron capture. For some of these, there are no values of E_β readily available to practioners of nuclear medicine. Some of these radionuclides, though emitting no beta particles, can produce a substantial on-site absorbed dose by conversion and Auger electrons and by relatively large amounts of low energy x-rays.

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In recognition of this, Loevinger *et al* (1) provided simple expressions by which the on-site absorbed dose from electron capture decay and conversion electrons may be calculated from nuclear decay scheme data. These expressions are quite adequate for most radionuclides, especially those emitting beta particles. Even for most electron capture decay processes, they yield only slightly low values. For a few cases, including that of the decay of mercury-197, they lead to a substantial error and must be modified.

We have developed more complete equations for the calculation of the total "beta-type" energy deposition that are extensions of Loevinger's expressions. While not significantly more accurate for many radionuclides, they are very useful for electron capture radionuclides. One advantage is that they facilitate computation of the photon yield, whether the photons be gamma rays or x-rays. This is helpful not only in calclulating photon yields for radionuclide calibration purposes, but also in calculating Γ, the specific gamma-ray constant.

It is realized that for most radionuclides the uncertainities of absorbed dose calculations of internally administered radionuclides are far greater than the uncertainities in values of E_β. We believe that it would be useful to derive more complete values, compatible with the photon yield, if only to prevent gross errors with a few nuclides. Moreover, there is every reason to believe that improved methods of absorbed dose calculation will soon be developed.

We propose that the symbol E_β be used for "the total local energy deposition per disintegration", and that

$$E_\beta \equiv \bar{E}_{\beta-} + \bar{E}_{\beta+} + E_e + E_p + E_\epsilon \qquad (1)$$

where $\bar{E}_{\beta-}$ and $\bar{E}_{\beta+}$ represent the average beta particle energy per distintegration for electrons and positions, respectively, and where E_ϵ and E_e represent the total local energy deposition due to electron capture and internal conversion processes, respectively. E_p represents local energy deposition due to photons of energy of 11.3 keV or less, not already included in E_ϵ or E_e.

The energy, 11.3 keV, was proposed by Loevinger *et al* (1) as the upper limit of the energy of photons which may be considered as depositing their energy locally. Photons of this energy lose 95% of their energy in water within 10 mm of the site of their emission. This is approximately the equivalent of the range of beta particles from phosphorus—32 in water.

Our values of E_β for several radionuclides of current interest are shown in Table I. The various terms defined in Eq. 1 are given to show the contributions of each. The derivation of the expressions used for computing values tabulated as well as general information on the electron capture and internal conversion processes is given in the Appendix. The photon yields from these same radionuclides, and values of Γ, the specific gamma-ray constant, are given in Table II.

DISCUSSION

Accounting for absorbed dose from fluorescent x-rays can be an especially perplexing problem. Where the energy of these rays is very low, *e.g.* K x-rays from the decay of chromium—51 at about 5 keV, the energy is expended over a very small range in tissue, and can easily be classed as "beta-like" energy depo-

TABLE I

VALUES OF E_β FOR SEVERAL RADIONUCLIDES

(Energies are in keV)

Radionuclide	$T_{1/2}$	$\bar{E}_\beta$	E_ϵ	E_e	E_p	E_β
Cesium-131	9.7 d	—	7.4	—	—	7.4†
Chromium-51	28. d	—	6.1	neg.	—	6.1
Cobalt-57	267. d	—	6.6	16.3	—	22.9
Iodine-125	60.2 d	—	7.1	13.7	—	20.8
Mercury-197	64.2 h	—	13.4	66.	—	79.4
Mercury-203	47. d	57.5	—	41.4	—	99.
Selenium-75	120. d	—	10.8	8.4	—	19.2
Strontium-85	65. d	—	6.4	7.7	—	15.1
Strontium-87m	2.8 h	—	—	81.	—	81. , 82.3*
Technetium-99m	6. h	—	—	12.	2.	14. , 14.8**

†Includes no component from K x-rays

*E_β, if 1.3 keV from ~ 15 keV K x-rays included as "on-site" deposition

**E_β, if 0.8 keV from ~ 19 keV K x-rays included as "on-site" deposition

sition. If the energy of the x-rays is high, *e.g.* the 68 and 78 keV K x-rays from the decay of mercury-197, one may consider accounting for this in terms of conventional gamma ray dose calculations.

Fluorescent x-rays between these energies present a real problem. Consider the K x-rays from the decay of strontium-85, strontium-87m and technetium-99m. They expend most, but not all, of their energy in one cm or less of tissue and produce a certain amount of "beta-like" energy deposition. They are, however, energetic enough to produce some absorbed dose over 2 cm away from their origin. To call them entirely "beta-like" is probably not correct. To include them in Γ leads to artificially inflated values of Γ.

K. Z. Morgan (2) includes in his values for $\bar{E}$, a term for the energy deposited in a chosen path length in tissue by a beam of escaping photons. The term is $E_\gamma(1-e^{-\sigma x})$, where σ is the total cross-section less σ_s, the Compton scattering cross section. When the range of interest is one cm or less, and the photon energy is over 50 keV, failure to include such a term results in negligible error.

For strontium-85 and strontium-87m, there is no serious problem because the contribution to absorbed dose by the K x-rays is small compared to other decay products. Of the two choices, including this energy in E_β is probably more reasonable. In making absorbed dose calculations for these radionuclides, however, the newer methods of Ellett *et al* (3, 4) and Snyder (5) which use Monte Carlo method are much to be preferred. These absorbed dose calculation methods make unnecessary the $(1-e^{-\sigma x})$ term, and eliminate the problem of the use of Γ at low energies.

TABLE II

PHOTON YIELDS (PER 100 DISINTEGRATIONS) AND VALUES OF Γ, SPECIFIC GAMMA-RAY CONSTANT (R-cm²/mc-hr)†
(Energies in keV)

Radionuclide	*Photon Type*	*Photon Energy*	*Number Per 100 dis.*		Γᵢ†	Γ†
Cesium-131	X, Kα	29.7	60.	75.	0.47	0.56*
	X, Kβ	33.7	15.		0.09	
Chromium-51	γ	323.	9.		0.15	0.15
Cobalt-57	γ	122.	87.5	96.3	0.46	
	γ	136.	8.8		0.05	
	γ	14.4	8.6		0.48	0.99
Iodine-125	X, Kα	27.4	112.6		1.02	
	X, Kβ	31.1	24.2	144.	0.17	
	γ	35.4	7.		0.04	1.23
Mercury-197	X, Kα	68.2	57.		0.18	
	X, Kβ	78.8	18.	94.	0.13	
	γ	77.3	20.			
	γ	191.	<0.1		——	0.31
Mercury-203	γ	279.	81.5		1.16	
	X, Kα	72.2	9.1	12.7	0.04	
	X, Kβ	82.4	3.6			1.20
Selenium-75	γ	265.	53.	81.	1.11	
	γ	280.	28.			
	γ	136.	40.	53.2	0.31	
	γ	121.	13.2			
	γ	402.	15.2		0.32	
	γ	97.	3.3		0.02	
	Others	——	4.7		<0.01	1.76
Strontium-85	γ	514.	99.2		2.69	2.69
Strontium-87m	γ	388.	78.2		1.60	
	X, Kα	14.	9.8	12.2	0.25*	
	X, Kβ	16.	2.4			1.85*
Technetium-99m	γ	140.	90.	90.4	0.56	
	γ	142.	0.4			
	X, Kα	18.3	4.6		0.16*	
	X, Kβ	20.6	1.1			0.72*

*See Table 1
†Γ calculated at 20° C.

Nuclides such as cesium-131 and iodine-125 are the most difficult to handle. Their fluorescent K x-rays are the "signal" radiation, but produce substantial amounts of "local" energy deposition. Accurate calculation of the gamma component of the absorbed dose for cesium-131 and iodine-125 may be made by the Monte Carlo method (3, 4, 5).

SUMMARY

Tabulated values of the average electron-type energy emitted per disintegration, the photon yields, and the specific gamma-ray constant are presented for the radionuclides ^{131}Cs, ^{51}Cr, ^{57}Co, ^{197}Hg, ^{203}Hg, ^{125}I, ^{75}Se, ^{85}Sr, ^{87m}Sr and ^{99m}Tc which are of current interest in nuclear medicine. Our method of calculating these parameters directly from nuclear decay scheme data is described in the Appendix.

APPENDIX

ELECTRON CAPTURE

When a radionuclide decays by electron capture, a vacancy is created in an orbital electron shell. This vacancy is almost immediately filled by an electron from an orbital level of a higher energy. The loss of energy due to this transition is accounted for by energy carried away from the atom either as x-ray photons or as Auger electrons. The x-ray photons have quantized energies characteristic of the daughter nuclide. Each Auger electron has an energy equal to the difference between the energy lost in the transition, and the energy binding it to the atom in its original shell. The ejection of one Auger electron leads to a second electron shell vacancy and to further electron transitions which, in turn, generate other x-ray photons or eject other Auger electrons.

The fraction of transitions in which the energy is carried away by x-ray photons is called the "fluorescent yield," ω. For each shell and for each different atom there exists a specific fluorescence yield. For example, the fraction of K x-rays emitted for each K-shell vacancy is designated as ω_K. This has a value which ranges from 0.966 for uranium to 0.049 for sulfur. For each K-shell vacancy, then, there will be ω_K K x-rays and $(1 - \omega_K)$ Auger electrons radiated. Each $K\beta$ x-ray will produce a vacancy in the L_{II} or L_{III} shells; these vacancies will then give rise to the release of L x-rays or Auger electrons or both. The energy carried away by the radiations resulting from an L-shell vacancy will be equal to the L-shell binding energy. This, generally, is sufficiently small as to be considered as electron-type radiation. $K\beta$ x-ray transitions are associated with the formation of vacancies in the M and N shells. Transitions of orbital electrons filling these vacancies lead to the release of local dose radiations having a total energy equal to the binding energy of the M (or N) shell.

Existing data gives fluorescent yields for L and M shells, but we shall need to use in our calculations only the yield for the K shell, ω_K, because L and M x-rays for atoms of atomic number, Z, less than 82 have energies less than 11.3 keV. For atoms of Z less than 35, K x-rays have energies near or less than 11.3 keV. As has been pointed out above, in such cases, one may consider the emitted radiation as locally deposited in the surrounding tissue. (The K x-rays of As

and Se and the L x-rays of Pb have energies slightly greater than 11.3 keV. There is no sharp change in the absorption of photons in the tissue at 11.3 keV. In computations reported here, these x-rays are treated as "electron-type" quanta).

Previous calculations assumed that all K x-rays were Kα. It is more accurate to use the Kα and Kβ yields. This is particularly true at high atomic numbers where K x-rays comprise a major part of the photon yield, and L x-rays contribute a large share of the local energy deposition.

For atomic numbers between 35 and 82, the component of local energy deposition caused by the L and M vacancies resulting in the production of K x-rays is given by:

$$k_K \omega_K \left[\frac{K\alpha}{K\alpha + K\beta} E_{L_{II-III}} + \frac{K\beta}{K\alpha + K\beta} E_{M_{II-III}} \right] \quad (2)$$

where the terms are defined in Table III

The ratios of

$$\frac{K\alpha}{K\alpha + K\beta} \text{ and } \frac{K\beta}{K\alpha + K\beta}$$

are the relative abundances of the Kα and Kβ x-rays respectively.

The values of 0.75 and 0.25 may be used for these ratios with reasonable accuracy in the range of Z from 35 to 82. Where greater accuracy is desired, as in the calculations for mercury-197, they may be found in *Nuclear Spectroscopy Tables*, page 81 (6). Since L and M binding energies are used, there is no need to compute L and M x-rays and Auger electron yields.

TABLE III

NOMENCLATURE

E_β	Total local energy deposition per disintegration (MeV/dis.).
E_ϵ	Local energy deposition per disintegration due to electron capture and subsequent products (MeV/dis.).
E_e	Local energy deposition per disintegration due to conversion electrons and subsequent products (MeV/dis.).
E_p	Local energy deposition per disintegration due to gamma-rays of energy less than 11.3 keV. (MeV/dis.).
k_K, k_L, k_M	Fractions of disintegrations that occur by K, L, and M capture, respectively.
E_K, E_{L_I}	Binding energies of K and L_I electron shells, respectively (MeV.).
$E_{I_{II-III}}$, $E_{M_{II-III}}$	Average of binding energies of L_{II} and L_{III}, and M_{II} and M_{III} electron shells respectively, (MeV.).
ω_K	K fluorescent yield.
f	Fraction of disintegrations giving rise to a photon of energy $E\gamma$
N_{e_K}, N_{e_L} ...	Number of K, L, . . . conversion electrons respectively arising from a photon of energy $E\gamma$ per disintegration.
α	Internal conversion coefficient.

The energy contribution associated with Auger electrons includes K Auger electrons, subsequent L or M Auger electrons, and the attendant low energy x-rays. This is given by

$$k_K\ (1 - \omega_K)\ E_K \tag{3}$$

The Kα and the Kβ x-ray yields are given by

$$k_K\omega_K \frac{K\alpha}{K\alpha + K\beta} \text{ and } k_K\omega_K \frac{K\beta}{K\alpha + K\beta}$$

Electron capture can involve, in addition to K capture as treated above, capture of electrons from the L_I, L_{II}, and M_I shells.

Terms representing the energy locally deposited as a result of these events are

$$k_{L_I} E_{L_I} + (k_{L_{II}} E_{L_{II}} + k_{M_I} E_{M_I})^{\dagger} \tag{4}$$

The fractions k_K, k_{L_I}, $K_{L_{II}}$ and k_M may be determined from K/L/M capture ratios and electron capture branching ratios given in Nuclear Data Sheets. When it is energetically possible, positron emission competes with electron capture. In this event, one must take into account the branching ratio between electron capture and positron emission in calculating k.

By combining equations (2), (3), and (4), one may obtain for the local energy deposited per disintegration due to electron capture

$$E_\epsilon = k_K\omega_K \left[\frac{K\alpha}{K\alpha + K\beta} E_{L_{II-III}} + \frac{K\beta}{K\alpha + K\beta} E_{M_{II-III}} \right] + k_K\ (1 - \omega_K)\ E_K + k_{L_I} E_{L_I} + k_{L_{II}} E_{L_{II}} + k_M E_M \tag{5}$$

for Z between 35 and 82. For Z less than 35, Equation (5) reduces to:

$$E_\epsilon = k_K E_K + k_L E_L \tag{5A.}$$

Some radionuclides can decay by electron capture to more than one energy state, as competitive processes. This must be considered in the capture branching ratios, and each transition calculated separately.

Then $$E_\epsilon = E_{\epsilon_1} + E_{\epsilon_2} + \ldots \tag{6}$$

Values for ω_K are given by Wapstra *et al* (6), and by Slack and Way (7). Electron shell binding energies are given by Hill, Church, and Mihelich (8) or by Wapstra *et al* (6).

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†If the energy of the electron capture transition exceeds the K-shell binding energy, K capture is most likely. Capture from the L_I shell is the next most likely. In nuclei of atomic number up to 50, and in allowed and first forbidden transitions, capture occurs almost entirely from these two shells. At high atomic number and where the binding energy of a shell is large compared to, but less than, the transition energy, significant numbers of captures involving the L_{II} and M shells will occur. This happens even in allowed and first forbidden transitions. The decay of mercury-197 is such an example; the table on page 61 of *Nuclear Spectroscopy Tables* (6) is very useful. Failure to account properly for L_{II} and M captures may result in an erroneous K x-ray yield.

INTERNAL CONVERSION

Internal conversion is a process that is competitive with gamma emission. In this process a nucleus loses excitation energy not by gamma emission, but instead by a transfer of energy to an orbital electron. Such a "conversion electron" is monoenergetic and is ejected from the atom. Its kinetic energy is equal to the energy of the gamma-ray (that might have appeared) less the binding energy of the shell from which the electron was ejected.

The relative occurrence of conversion is given by the conversion coefficient, α, which is the electron to gamma ratio ($N_e/N\gamma$). Internal conversion is most probable in the innermost electron shells, K, L, M . . . There will be a conversion coefficient for each shell and

$$\alpha_t = \alpha_K + \alpha_L + \alpha_M + \ldots$$

Vacancies in the shells caused by internal conversion are filled as discussed under electron capture, resulting in x-rays and Auger electrons. (In the Nuclear Data Sheets α_t is given as α.)

The number of K, L, and MN . . . conversion electrons respectively arising from a photon of energy $E\gamma$ per disintegration will be described as N_{e_K}, N_{e_L}, N_{e_M}, . . ., and

$$N_{eK} = \frac{\alpha_K}{1 + \alpha_t}, N_{eL} = \frac{\alpha_L}{1 + \alpha_t}, N_{eM} = \frac{\alpha_M}{1 + \alpha_t}$$

(Note: In many instances the Nuclear Data Sheets will give α_K or α_t, and the K/L/MN ratios, or the numerical ratios of K conversion electrons to L conversion electrons to M conversion electrons. These data are usually sufficient for calculating N_e.)

The contribution to local energy deposition is given as:

$$\begin{aligned} E_e = {} & fN_{eK}(E\gamma - E_K) + fN_{eL}E\gamma - fN_{eM}E\gamma \\ & + fN_{eK}(1 - \omega_K)E_K \\ & + fN_{eK}\omega_K\left[\frac{K\alpha}{K\alpha + K\beta}E_{L_{\text{II-III}}} + \frac{K\beta}{K\alpha + K\beta}E_{M_{\text{II-III}}}\right] \end{aligned} \quad (7)$$

The terms on the first line give the direct contributions of the conversion electrons from the K, L, and M shells respectively. The term on the second line gives the contribution of K Auger electrons following K conversion. The term on the third line states the contribution of L and lower order x-rays and Auger electrons resulting in K x-ray emission following K conversion. The fraction of disintegrations giving rise to a photon of energy $E\gamma$ is given by f.

Equation 7 may be simplified, by combining of terms, to:

$$\begin{aligned} E_e = {} & fN_{eK}\left[E\gamma - \omega_K E_K + \omega_K\left\{\frac{K\alpha}{K\alpha + K\beta}E_{L_{\text{II-III}}} + \frac{K\beta}{K\alpha + K\beta}E_{M_{\text{II-III}}}\right\}\right] \\ & + E\gamma\,(fN_{eL} + fN_{eM} + \ldots) \end{aligned} \quad (8)$$

For $Z < 35$, *Eq.* 8 reduces to $E_e = (fN_{eK} + fN_{eL} + \ldots)E\gamma$,

$$\text{or } E = {}_e f N_{e_i} E_\gamma, \text{ or } E_e = f \frac{a_i}{1 + a_i} E_\gamma \tag{8.1}$$

As in the situation of more than one electron capture, the effects of internal conversion of additional gamma-rays in the same or competitive decay processes are summed.

Then $$E_e = E_{e_1} + E_{e_2} + \ldots \tag{9}$$

The photon yield, or the number of unconverted photons, is given simply by:

$$f\left(\frac{1}{1 + a_i}\right) \tag{10}$$

LOW ENERGY PHOTONS

It is seen that in the foregoing development, the low energy x-rays associated with electron capture and internal conversion were included in the local energy deposition. In the decay of some nuclides, very low energy gamma rays are emitted, and if their energy is less than 11.3 keV, they must be treated as "electrons". For example, in the decay of ^{99m}Tc, a 2 keV gamma ray is emitted. The term E_p provides a place to insert the energy of such emissions, and is given by:

$$Ep = fE_\gamma, \text{ for } E_\gamma \leqslant 11.3 \; keV \tag{11}$$

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