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CALCULATED DISTANCE DISTRIBUTIONS OF ENERGY TRANSFER EVENTS IN IRRADIATED LIQUID WATER*

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Abstract. Histories from a Monte Carlo electron transport calculation in liquid water are analyzed to obtain the distance distribution functions, t(x) and T(x), of energy transfer events. These functions, which give the average energy transferred within a distance x from an arbitrary transfer event, are presented for irradiation by monoenergetic electrons of several energies between 500 eV and 1 MeV, for monoenergetic photons of 10, 50, and 200 keV energy and for 65 kVp and 200 kVp x rays and ^{60}Co γ rays. The dose average lineal energy in spherical sites as a function of site radius is also presented for these same photon spectra.

1. Introduction

The initial pattern of energy deposition in irradiated matter is the starting point for many models of radiation effects. These models are aimed at understanding and predicting effects such as cell killing, for example, for cases which may include high LET radiations or low doses. Traditionally, "classical" microdosimetry has been concerned with the distributions of absorbed energy and related quantities in micron-sized volume elements. Recently it has become increasingly apparent that not only the distribution of energy deposited, but also the correlation between energy loss events, such as ionizations, or between initial products formed, such as OH radicals, may be of great importance in determining radiation effects. As an example, it is well known that for producing many biological end points, the radiation from ^{60}Co is less effective than that from lower energy x rays. Yet calculations indicate that the spectrum of slowing-down electrons, except at high energies, is identical for the two cases.[1] Differences in correlations between loss

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events is a possible explanation. Another area in which correlations may be of importance is in radiation effects in microelectronics components in orbiting satellites.[2] A sufficient concentration of ionization in a critical volume may produce an error in a computer memory. The subject of this paper is the calculation of certain correlations between energy transfer events in irradiated liquid water.

2. The Functions t(x) and T(x)

Kellerer and co-workers have introduced a function which they refer to as the distance distribution of energy transfers.[3] If a transfer point is randomly chosen, then the expected energy imparted within a distance x of the point is T(x). If ϵ_i is the energy transferred at point i, then the contribution to T(x) from a single particle track is

$$T(x) = \frac{\sum_{(i,j)<x} \epsilon_i \epsilon_j}{\sum_i \epsilon_i} , \tag{1}$$

where the sum in the numerator extends over all pairs of transfer points such that their separation is less than x. [There is an additional contribution to T(x) due to independent particle tracks, but it is trivially proportional to dose. In what follows we shall only be concerned with the single-track contribution to T(x)].

The function t(x) is the differential distribution

$$t(x) = \frac{dT(x)}{dx} . \tag{2}$$

Since T(x) is the average energy transferred within a sphere of radius x about a transfer point, it has a direct application to radiation effects models in which a given amount of energy within a sensitive site is needed to produce a given effect. However, these functions may also be used to calculate some of the familiar quantities of microdosimetry. As one example, we quote the formula given by Kellerer and Chmelevsky[3] for the dose average of lineal energy in a spherical site of radius r,

$$\bar{y}_D = \frac{3}{4r} \int_0^{2r} \left(1 - \frac{3x}{4r} + \frac{x^3}{16r^3}\right) t(x)dx . \tag{3}$$

3. Calculations and Results

We have previously reported results from a Monte Carlo electron transport code for liquid water.[4] This code incorporates cross sections appropriate for the condensed phase and includes collective effects *a priori* by use of the dielectric response function. It transports the electrons event-by-event and includes various ionization and excitation events as well as elastic scattering. Each primary electron and all of the secondaries produced are transported until they fall below a cutoff energy (10 eV in this calculation). Such a transport calculation is an ideal starting place to obtain the distance distribution of energy transfers, since complete details are known at each transfer point.

The transport code was run for each of several initial electron energies, and the histories, containing full information about every energy transfer event--coordinates, energy transferred and type of event, were stored in data files. These files were then read and the histories analyzed to obtain the T(x) and t(x) functions by evaluating Eqs. 1 and 2. For each event i, the distance x to every other event j is calculated and the product of energy transfers $\varepsilon_i \varepsilon_j$ is logged into pre-selected bins in distance x. For low energy primary electrons, the evaluation is straightforward; however, since the functions involve a double sum over the energy transfer events, the computing time goes as the square of the number of events and, hence, as the square of the primary electron energy. For a 1 MeV electron, there are more than 70,000 events. In order to make the calculation possible, some means for reducing the amount of computation was necessary. The events were read in sequence along the electron track in blocks of 500 events, for example. A rectangular parallelepiped was determined by their coordinates and only the events in that block and others within a given distance (usually 10μm) from the parallelepiped were considered in the sum. Thus, very distant correlations were not considered and the computing time was correspondingly reduced. As a further means to reduce the computing time for the higher energies, only some of the events (e.g., 10%) were selected, randomly, to be paired with the other events.

Results of the calculations for 100 keV electrons are shown in Fig. 1. The solid curves show the t(x) and T(x) functions which result

when all energy loss events are considered. In this calculation when an electron loses energy and falls below cutoff, its energy is added to that of the ionization or excitation event in which the energy loss occurred. The dashed curves are obtained by considering only ionization events. T(0) is simply the average energy of an energy loss event: about 11 eV for an ionization and about 14 eV when all events are considered (this includes the average energy of the subexcitation electron). The solid curve for T(x) has a value of 265 eV at x = 20 nm. This is the average energy which is deposited by events resulting from the same primary particle within a 20 nm radius sphere around an arbitrary energy loss event when water is irradiated by 100 keV electrons. Figure 2 shows results for several different electron energies. In each case these are the averages obtained when a primary electron of given energy and all its secondaries slow down in liquid water. These curves are calculated by considering all energy loss events as for the solid curves in Fig. 1. All the curves approach virtually the same value for very small x, the average energy loss per event, which is nearly independent of the initial electron energy. For large enough values of x, each curve would reach a value equal to the initial energy of the electrons, since that total energy would be deposited in a large sphere around any arbitrary loss event.

In order to calculate the distance distributions for water irradiated by photons, we used the code PHOEL-2 which gives the initial spectrum of electrons produced in water by photons.[5] The values of T(x) calculated for several electron energies were then averaged over the appropriate electron spectrum from PHOEL-2. An actual sample of electrons from the part of the spectrum produced with energies less than 2 keV were transported and analyzed to give the contributions from these electrons for each case. The results for three x-ray energies are shown in Fig. 3. The dashed curves are for the electron distribution which results when the photon is allowed to Compton scatter (or possibly produce a photoelectron) only once. The solid curves result when the photon is allowed to repeatedly Compton scatter until it is eventually absorbed in producing a photoelectron.

In general, the lower energy photons have a softer electron spectrum and thus, by reference to Fig. 2, would be expected to have a greater average energy absorbed within a given distance around an energy loss event. Allowing successive Compton scatters produces a more similar initial electron spectrum from the 200 keV and 50 keV x rays and thus the T(x) are more nearly the same than for the single scatter case.

Calculations were also made for several photon spectra, and the results for T(x) are presented in Fig. 4 and in the following table.

Distance Distribution of Energy Transfer Events, T(x), in eV

Radiation	Distance, x, in nm						
	0.3	1	3	10	15	30	100
65 kVp x rays	14.9	22.4	59.6	191	274	480	1130
200 kVp x rays	15.0	22.6	60.4	194	280	497	1190
^{60}Co with single Compton scattering	14.9	20.3	47.0	141	196	310	570
^{60}Co with multiple Compton scattering	14.9	21.0	50.2	151	210	340	674

The 200 kVp x-ray spectrum which we used is that given by Cormack and Johns[6] and is based on measurements by Greening.[7] The 65 kVp spectrum was reported by Fewell and Shuping[8] for a "typical" diagnostic x-ray beam with 1 mm of added Al filtration. The ^{60}Co spectrum contains equal numbers of photons with energies 1170 and 1330 keV.

The results for either the 200 kVp or the 65 kVp spectra were virtually the same whether single or multiple Compton scattering was considered. In the case of ^{60}Co, the multiple scattering gives a considerably softer spectrum; however, due to the large attenuation length for ^{60}Co photons, the single scatter spectrum is probably more realistic for nearly all irradiation arrangements. A clear difference appears between the ^{60}Co γ's and the lower energy x rays. Even for quite small spheres there is on the average more energy deposited around

a given energy loss event in the case of the x-ray irradiation than there is for the ^{60}Co. Thus, a model for radiation effects which postulates dependence on energy concentration in small sites would predict a greater effect for the x rays relative to ^{60}Co.

The dose mean lineal energy, $\bar{y}_D$, is calculated from Eq. 3 and is shown in Fig. 5 for these same radiations. Again, there is a clear difference between the ^{60}Co and the x rays. These results are for the single track contribution. The results when the contribution from uncorrelated dose from other tracks is added is indicated for a dose of 100 rad by the dashed branch on the upper curve in Fig. 5. This contribution goes as the square of the radius and thus, once it becomes appreciable, it very quickly becomes dominant as the radius increases. The contribution to the other curves is not shown, but would be similar.

4. Conclusion

We have presented Monte Carlo calculations of the single track contributions to the distance distribution function of energy transfers, T(x), and its derivative, t(x), in water irradiated by monoenergetic electrons and by various photon spectra. We have found differences in the average energy deposited around an energy loss event which may help to explain differences in effectiveness in producing radiation effects.

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FIGURE CAPTIONS

Fig. 1. Single-track contribution to distance distribution functions T(x) and t(x) of energy transfer events for 100 keV electrons. Solid curves are calculated for all energy transfer events, dashed curves for ionization events only.

Fig. 2. Single-track contribution to distance distribution function T(x) of energy transfer events for monoenergetic electrons of various initial energies.

Fig. 3. Single-track contribution to distance distribution function T(x) of energy transfer events for monoenergetic photons of several energies. Solid curves for electron spectra calculated assuming multiple Compton scatterings, dashed curves for single Compton scattering.

Fig. 4. Single-track contribution to distance distribution function T(x) of energy transfer events for various photon spectra.

Fig. 5. Single-track contribution to dose mean lineal energy $\bar{y}_D$ for various photon spectra. Dashed curve indicates inclusion of independent track contribution for a dose of 100 rad.

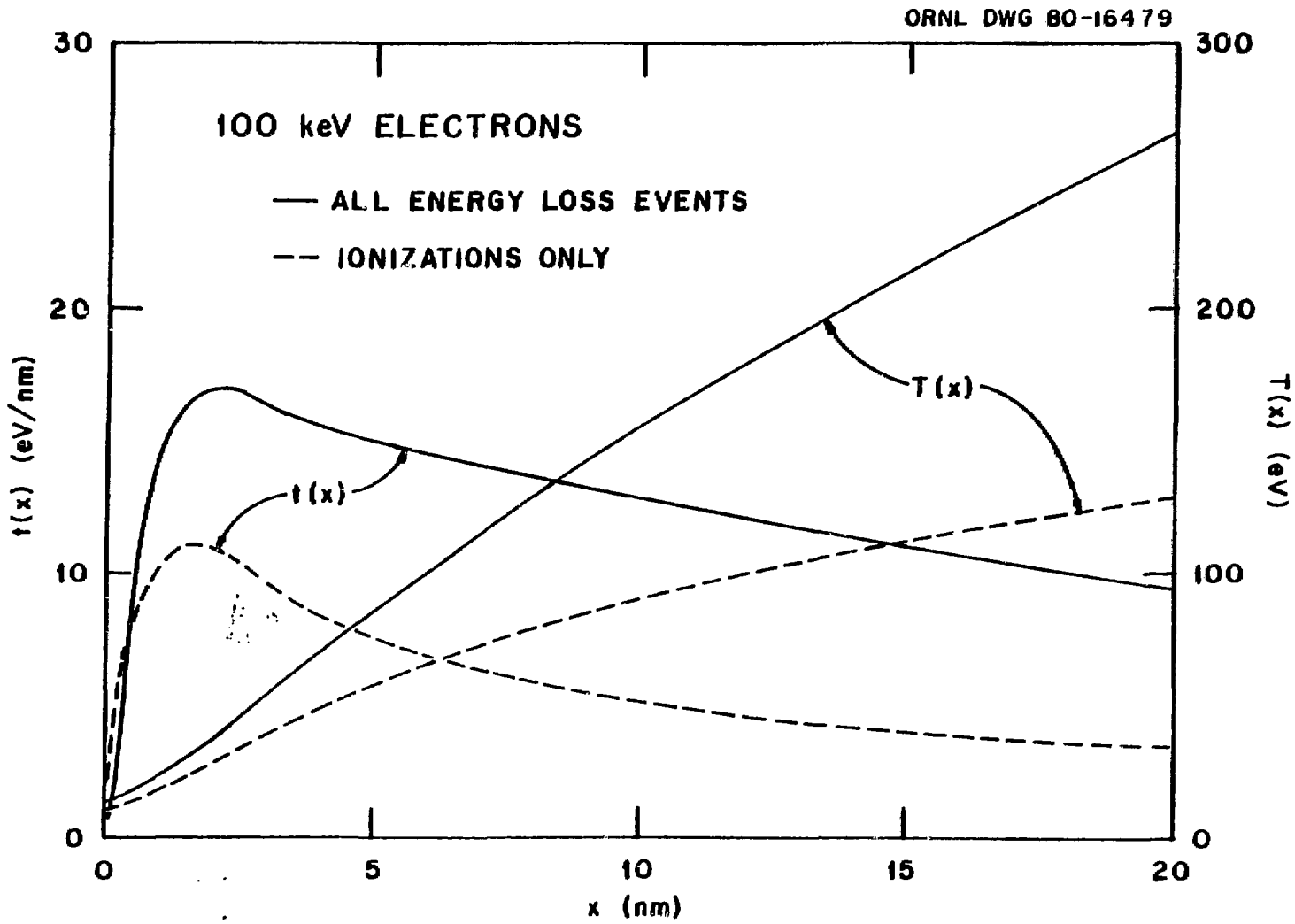

ORNL DWG 80-16479
100 keV ELECTRONS
— ALL ENERGY LOSS EVENTS
-- IONIZATIONS ONLY
t(x)
T(x)
t(x) (eV/nm)
T(x) (eV)
x (nm)
0
5
10
15
20
30
300
200
100

Figure 1

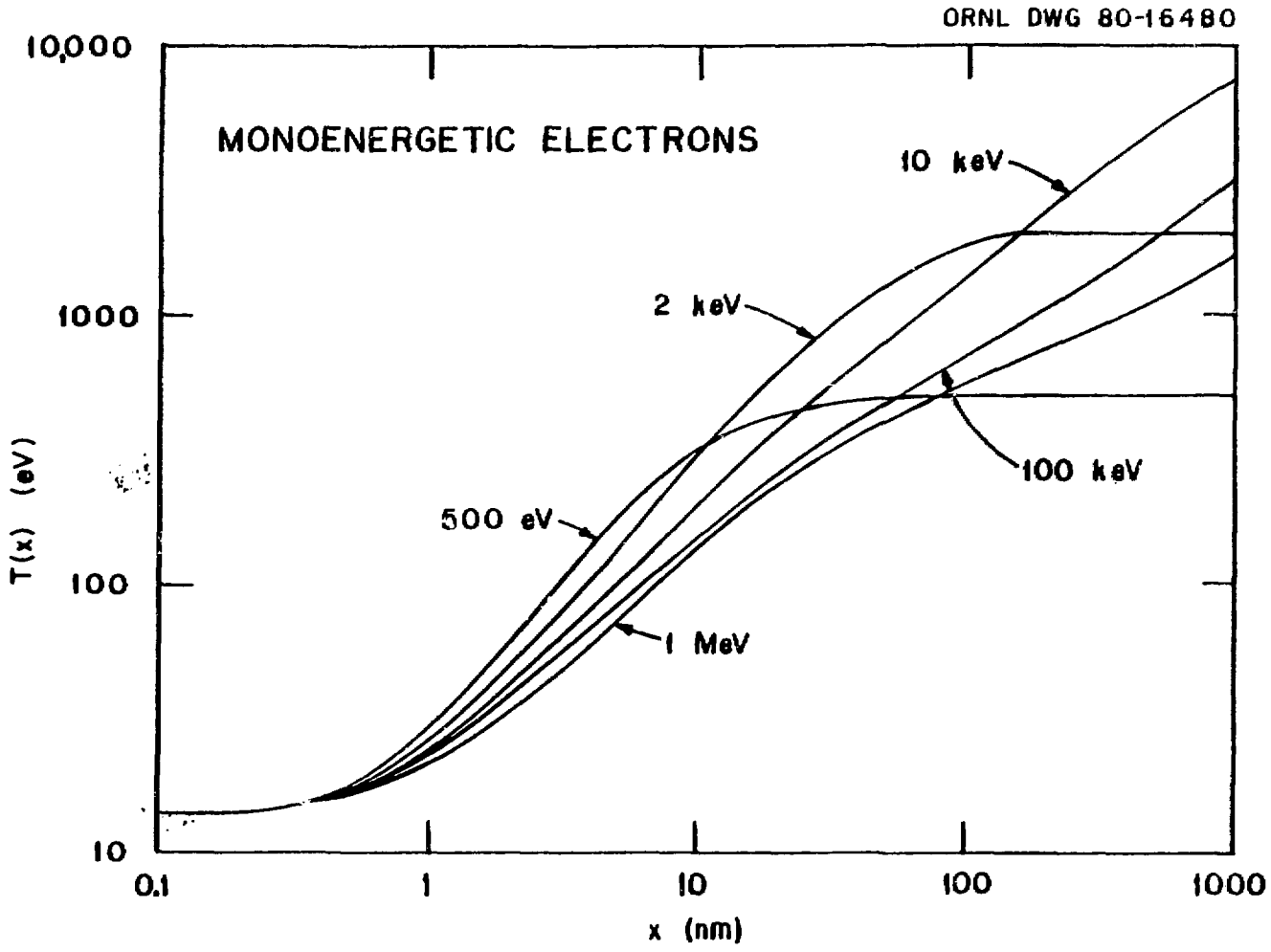

ORNL DWG 80-16480
MONOENERGETIC ELECTRONS
10 keV
2 keV
500 eV
100 keV
1 MeV
10,000
1000
100
10
T(x) (eV)
0.1
1
10
100
1000
x (nm)

Figure 2

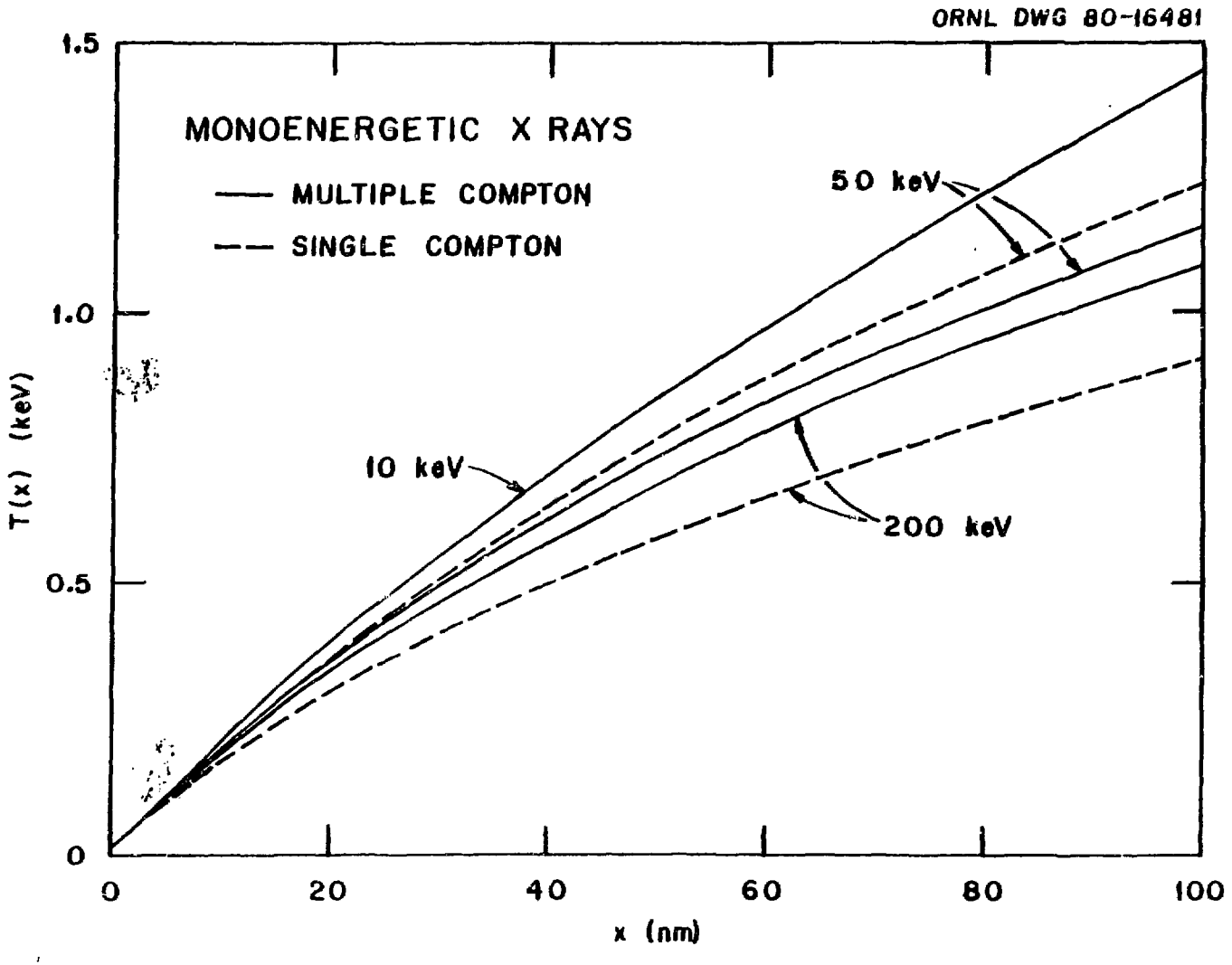
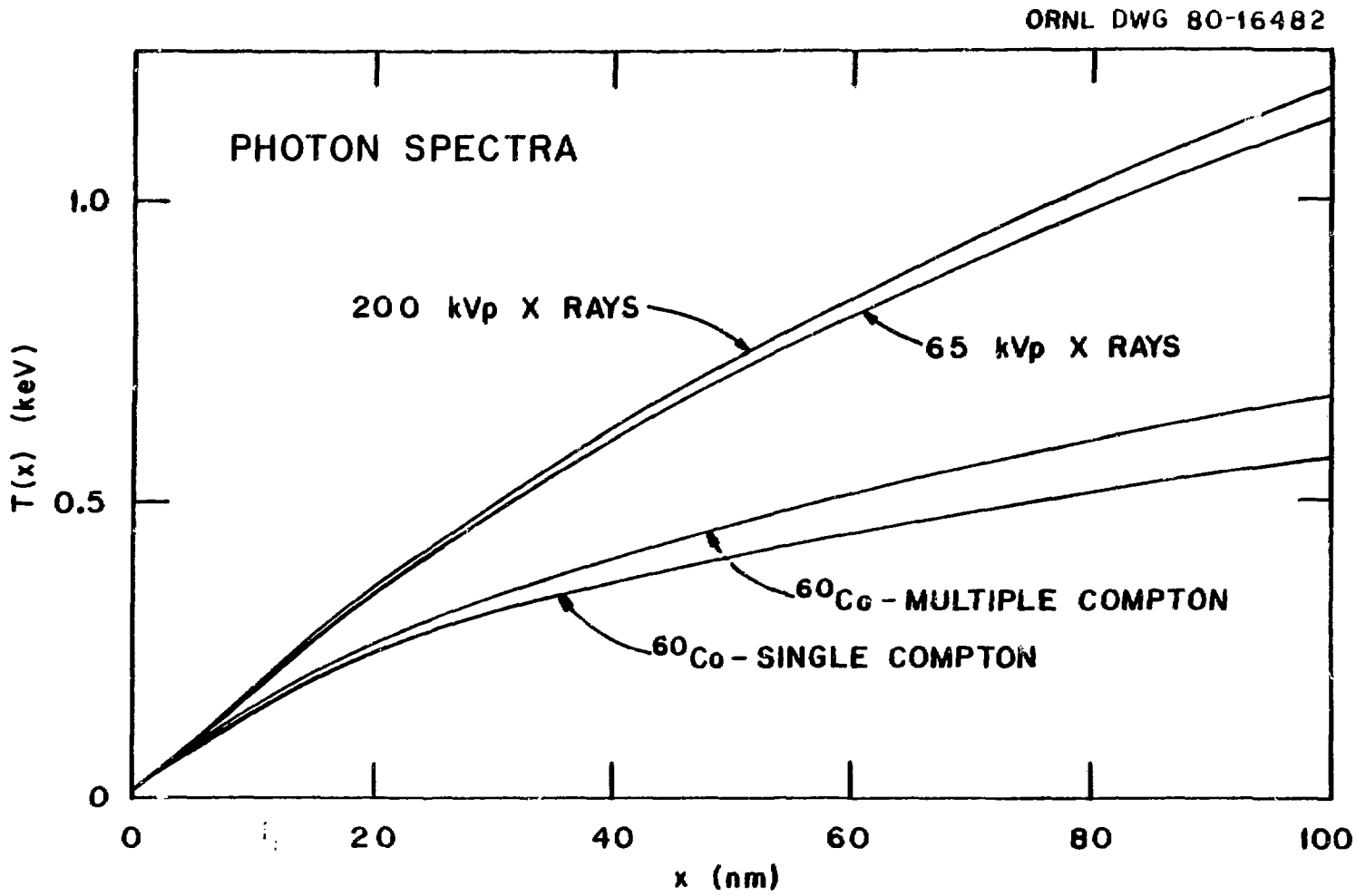

ORNL DWG 80-16481
MONOENERGETIC X RAYS
MULTIPLE COMPTON
SINGLE COMPTON
50 keV
10 keV
200 keV
T(x) (keV)
x (nm)
0
0.5
1.0
1.5
0
20
40
60
80
100

Figure 3

Figure 4


ORNL DWG 80-16482
PHOTON SPECTRA
1.0
0.5
0
T(x) (keV)
200 kVp X RAYS
65 kVp X RAYS
60Co - MULTIPLE COMPTON
60Co - SINGLE COMPTON
0
20
40
60
80
100
x (nm)

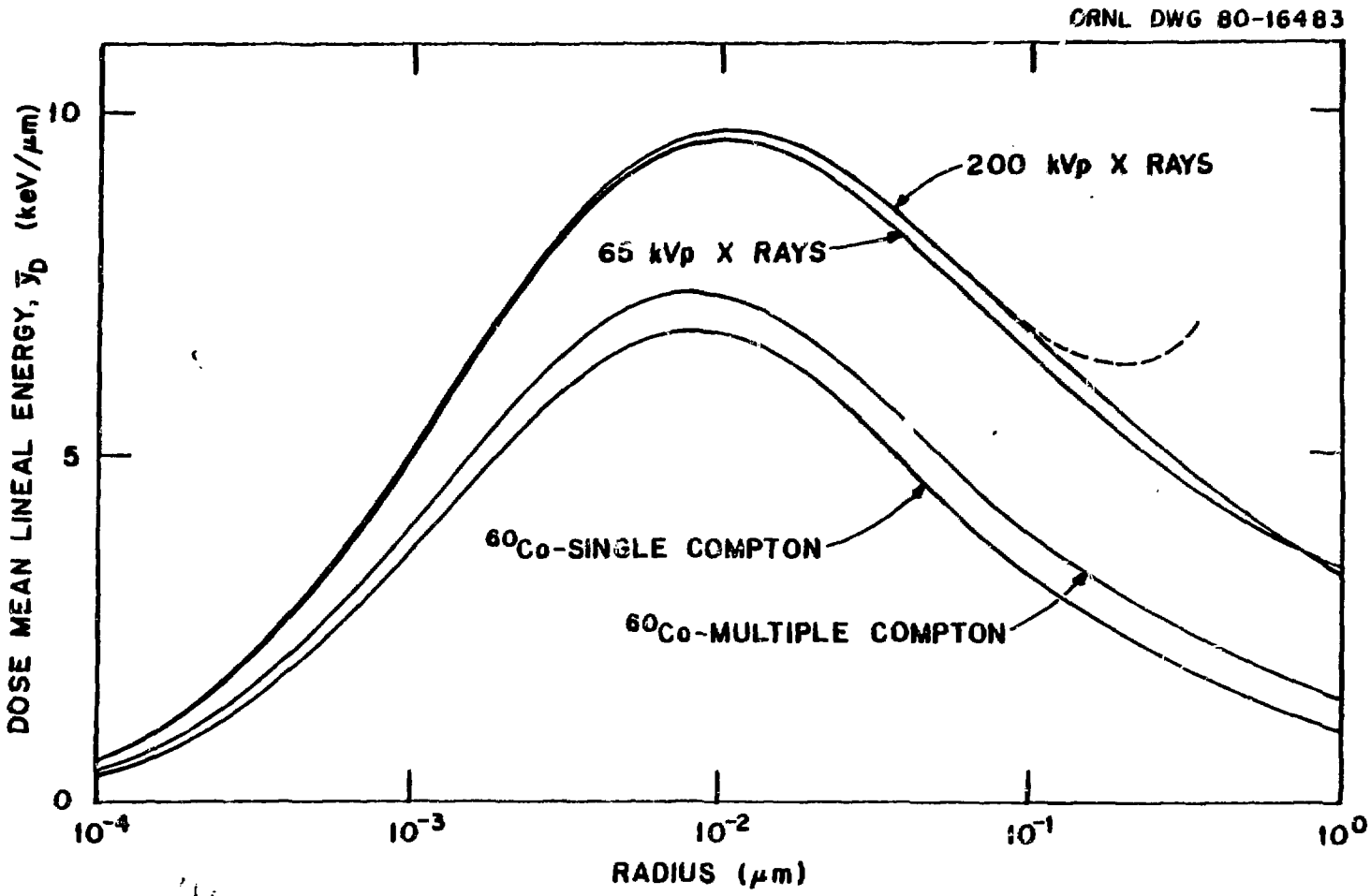

ORNL DWG 80-16483
DOSE MEAN LINEAL ENERGY, $\bar{y}_D$ (keV/μm)
10
5
0
200 kVp X RAYS
65 kVp X RAYS
^{60}Co-SINGLE COMPTON
^{60}Co-MULTIPLE COMPTON
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
RADIUS (μm)

Figure 5