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A User's Manual for ALDOSE: A Computer Code for Calculating Absorbed-Dose Rate, Dose-Equivalent Rate, and Dose-Weighted LET as Functions of Depth in Water Irradiated by an Alpha Disc Source

T. E. Huston
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A User's Manual for ALDOSE: A Computer Code for Calculating Absorbed-Dose Rate, Dose-Equivalent Rate, and Dose-Weighted LET as Functions of Depth in Water Irradiated by an Alpha Disc Source

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A User's Manual for ALDOSE: A Computer Code for Calculating Absorbed-Dose Rate, Dose-Equivalent Rate, and Dose-Weighted LET as Functions of Depth in Water Irradiated by an Alpha Disc Source

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I. ABSTRACT

ALDOSE is a Fortran computer code written to calculate the absorbed-dose rate, dose-equivalent rate, and dose-weighted LET as functions of depth in water irradiated by a uniform alpha disc source. In addition, the average LET and average quality factor for the irradiated water are computed. The program accommodates a source upon which a layer of gold may reside and which may be separated from the water by a sheet of Mylar. The presence of gold and/or Mylar is optional and must be specified by the user. ALDOSE can process a source having up to 12 alpha energies ($\leq$15 MeV) in its spectrum. Lateral dimensions of the source are assumed to be large when compared to alpha-particle ranges in water. Calculations are based on range-energy tables for alphas in gold, Mylar, and water and employ a technique of ray tracing. Output data are tabulated as histograms and graphs in files which can be accessed by the user for further processing and plotting.

II. INTRODUCTION

Many studies in radiobiological and radiochemical fields involve calculation of dosimetric quantities for soft tissue or water exposed to an alpha-emitting radioisotope. A Fortran program, ALDOSE, has been written to compute the absorbed-dose rate, dose-equivalent rate, and dose-weighted LET as functions of depth in water irradiated by a uniform, monolayer alpha disc source. To accommodate commercially-prepared sources, provisions allowing for the presence of a layer of gold upon the source have been made in the code. Furthermore, ALDOSE can handle an exposure system in which a sheet of Mylar has been placed between the source and the water. Both gold and Mylar layers are optional, and their presence in a system is specified by the user. A source possessing up to twelve alpha-particle energies (with a maximum energy of 15 MeV) in its spectrum can be processed by the program.

The lateral dimensions of the disc source are assumed to be large in comparison with the ranges (in water) of the alpha particles; thus, the quantities of interest depend only on the distance from the source. These quantities are calculated at various depths in the water between planes specified by the user (i.e., subslabs of water).

The computational technique is based on range-energy tables (Berger, 1990) of alpha particles in gold (19.32 g/cm^3), Mylar (1.38 g/cm^3), and water (1.00 g/cm^3), and involves tracing alpha-particle rays to determine energy deposition

within the user-specified subslabs of water. The program execution time depends on the emission energies and number of alpha tracks used in calculations. With a MicroVax II, several minutes of CPU time should be adequate for most applications.

III. COMPUTATIONAL METHOD

The computations of ALDOSE are performed for the geometry shown schematically in Fig. 1. The target medium consists of slabs of gold, Mylar, and water covering a monolayer alpha source. The water is divided into subslabs indicated by the dashed lines and begins at the plane Z=0. The user specifies whether the gold and/or Mylar are present, and ALDOSE places the source at the appropriate depth (e.g., for absence of both, source is placed on the plane Z=0, at the lower water surface). The angle θ with respect to the normal gives the direction of travel of an alpha particle emitted from the source.

For an alpha particle emitted with a given initial energy at an angle θ, ALDOSE uses range-energy tables to calculate the distances traveled and energies deposited within the gold, Mylar, and water subslabs until the alpha comes to rest. The program computes the average LET, given by the quotient of the energy deposited and distance traveled, within each subslab traversed by the alpha particle. Based on ICRP Publication 26 (1977), the average LET in a subslab is used to assign a quality factor for the dose that the alpha particle

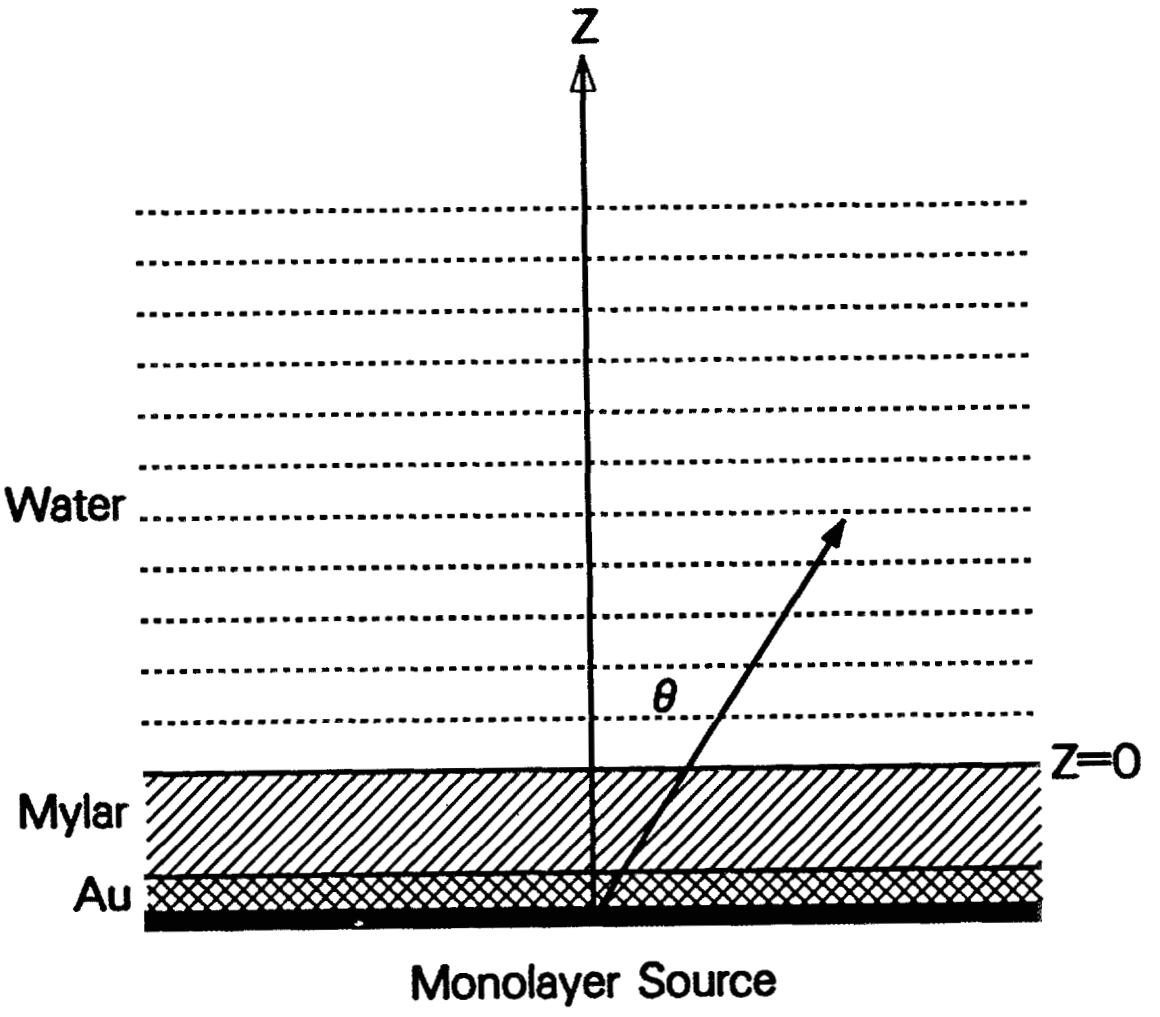

Fig. 1. Schematic diagram showing geometry used in calculations.

delivers there. The absorbed dose is proportional to the energy deposited, and the dose equivalent is proportional to the product of the quality factor and the energy deposited.

ALDOSE processes a number of alpha particles emitted isotropically from a point in the source to obtain the dose-weighted LET, average absorbed dose, and average dose equivalent per alpha in each subslab.

Since alpha particles are emitted isotropically from the disc source, a probability density function may be found for the angle θ. The probability that emission occurs between an angle θ and $\theta+d\theta$ is $P(\theta)d\theta=\sin\theta d\theta$, with $0\leq\theta\leq\pi/2$. The cumulative probability that an emission angle is not greater than θ is $P_c(\theta)=1-\cos\theta$. ALDOSE employs this expression to distribute the emission angles of N monoenergetic alpha particles by the following algorithm:

$$1-\cos\theta_i = (i-1)/N, \quad i = 1,2,3,...,N \tag{1}$$

where θ_i is the angle of the ith alpha particle. Figure 2 shows an example of the distribution of N=25 alpha particles emitted in the plane of the page (no gold or Mylar layers are present in this example). Note that the isotropic alpha particles tend to be emitted at angles θ which are close to the source plane in three dimensions.

When the source emits alpha particles of more than one energy, ALDOSE uses the emission frequencies to partition the total number of alpha particles used in calculations (i.e., parameter N) into smaller groups of monoenergetic

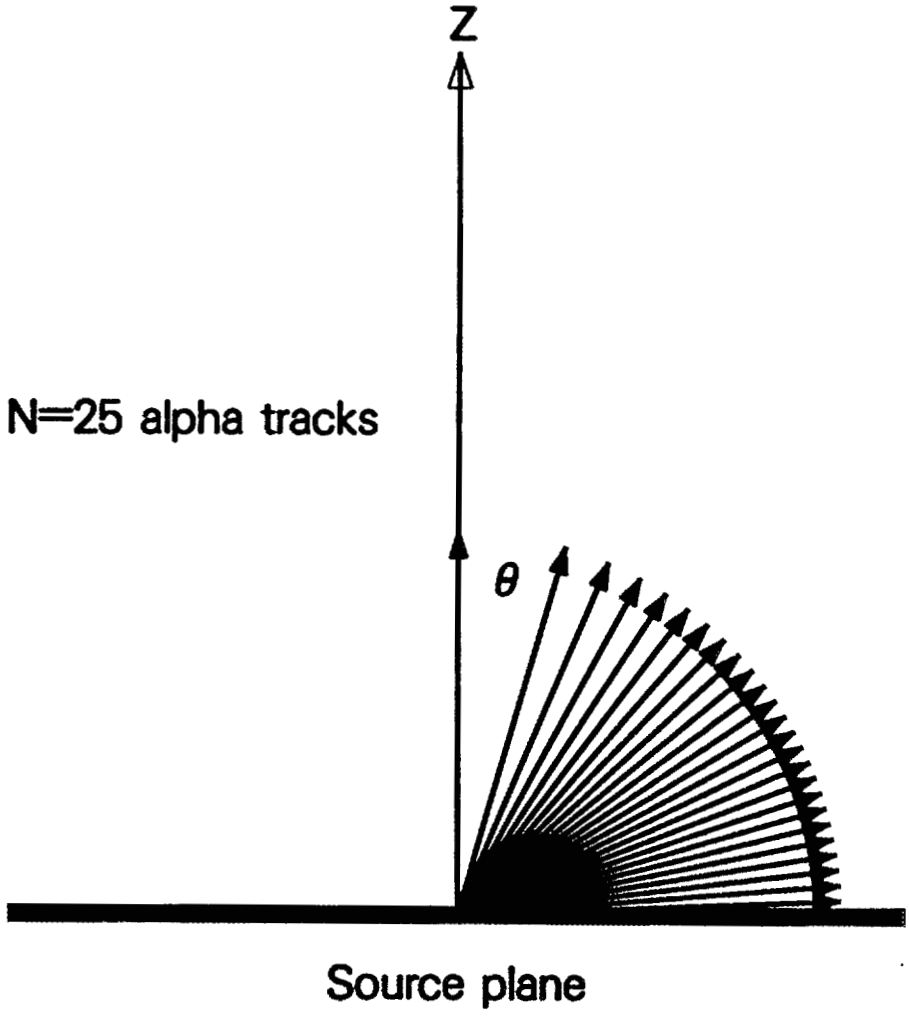

Fig. 2. Example of distribution in polar angle θ for N=25 alpha particles emitted isotropically from a point on the disc source.

particles. The above algorithm, Eq. (1), is then applied to each energy group to determine emission angles.

Using the dose and dose equivalent per alpha, as computed in subslabs irradiated by a number of isotropic alpha particles, ALDOSE calculates the dose rate (Gy/min) and dose-equivalent rate (Sv/min) in the subslabs for a disc source having a uniform activity density of 1 Bq/cm^2. (It is assumed that the source emits an average of 0.5 alpha particles $cm^{-2}s^{-1}$ in the "upward" direction, $\theta<\pi/2$.)

IV. USER INPUT PARAMETERS

ALDOSE reads input parameters from the file, ALDOSE.DAT, which is the only file to be edited by the user for his/her specific needs. The units MeV and μm are used throughout for energy and distance. The file is annotated at the bottom for help in editing. Table 1 lists all user-specified parameters in ALDOSE.DAT and the restrictions which apply to each. (A sample file of ALDOSE.DAT is shown in Table 2, Section VI of this manual.)

V. OUTPUT OF ALDOSE

Running ALDOSE creates two output files. The first, ALDOSE.OUT (unit=5), contains data echoed from the input file and the tabulated values of the absorbed-dose rate (Gy/min), dose-equivalent rate (Sv/min), and dose-weighted LET (keV/μm). One tabulation is in the form of a histogram with respect to slab

Table 1. User Input Parameters for ALDOSE

Parameter	Definition	Restrictions
N	Total number of alpha tracks used in calculations	Integer
NE	Number of alpha particles in source spectrum	Integer ≤ 12
EO(I)	Alpha energies (MeV) found in source spectrum	$EO(I) \leq 15.0$ $I=1,2,3,..,NE$
FRQ(I)	Alpha emission frequencies in source spectrum	$I=1,2,3,..,NE$
NSB	Total number of slab boundaries (planes) used in calculations	Integer ≤ 101
Z(I)	Depths (μm) of slab boundaries	$Z(I+1) \geq Z(I)$ $Z(3)=0$ (water interface). See note at bottom of ALDOSE.DAT (Section VI, Table 2)

boundaries; the second is in the form of a graph, with depths taken to be midway between the boundaries. The overall, average LET and quality factor for the volume of irradiated water are also given. The second file, DATA.OUT

(unit=6), contains only the numerical data sets necessary for plotting either a histogram or a graph. Data in this file can be read into an appropriate plotting code. Note that both rates are calculated for a source with uniform activity density of 1 Bq/cm^2. Also, slabs 1 and 2 are specific for gold and Mylar, respectively, in the output files. (A sample output file is shown in Table 3, Section VI.)

VI. SAMPLE RUN OF ALDOSE

A sample run of ALDOSE was made for a ^{226}Ra source. This nuclide emits two principal alpha particles with energies of 4.78 MeV (95%) and 4.60 MeV (5%). Calculations were performed for the geometry shown in Fig. 1 with a 0.0518 μm layer of gold followed by a 6.00 μm sheet of Mylar. Thus, the first three slab boundaries were Z(1)=-6.0518 μm, Z(2)=-6.00 μm, and Z(3)= 0.00 μm. A total of N=10,000 alpha particles were used in calculations.

The input file, ALDOSE.DAT, for this run is given in Table 2; the output file, ALDOSE.OUT, is shown in Table 3. The elapsed time, which was only slightly greater than the CPU time, is shown at the bottom of Table 3. Figures 3, 4, and 5, respectively, show plots of the absorbed-dose rate, the dose-equivalent rate, and the dose-weighted LET as functions of depth in water for the ^{226}Ra source. A comparison of the numerical results of this run (using N=10,000 alpha particles) with those of a run using N = 100,000 particles showed very little

difference. The average LET and quality factor in the irradiated water were found to be 167 keV/μm and 18.6, respectively.

Table 2. Sample input file, ALDOSE.DAT, for ^{226}Ra source

```
10000          2
4.78          .95
4.60          .05
55
-6.0518
-6.0000
 0.0     1.0     2.0     3.0     4.0     5.0
10.0    11.0    12.0    13.0    14.0    15.0    1
20.0    21.0    22.0    23.0    24.0    25.0    2
30.0    31.0    32.0    33.0    34.0    35.0    3
40.0    41.0    42.0    43.0    44.0    45.0    4
50.0   100.0  1000.0

N       NE                N=NUMBER OF ALPHA PAR
EO(1)    FRQ(1)           NE=NUMBER OF ALPHA PA
EO(2)    FRQ(2)           EO(I)=ITH ALPHA ENERG
.         .               FRQ(I)=FREQUENCY OF E
.         .
.         .
NSB                            NSB=NUMBER OF SLA
Z(1)                           Z(1)=DEPTH IN MIC
Z(2)                           Z(2)=DEPTH IN MICR
Z(3)    Z(4)     Z(5)   ...    Z(3)=0.0 (WATER IN
...     ...     ...   Z(NSB)   Z(I)=DEPTH IN MICR

NOTE:   SLAB ONE, Z(1) TO Z(2), IS SPECIFIC FOR
        SLAB TWO, Z(2) TO Z(3), IS SPECIFIC FOR

        1) IF GOLD IS NOT PRESENT, SET Z(1) EQUA
        2) IF MYLAR IS NOT PRESENT, SET Z(2) EQU
```

Table 3. Sample output file, ALDOSE.OUT, for ^{226}Ra source

DATE = 13-JUL-90

TIME = 15:20:32

NUMBER OF ALPHA ENERGIES IN SOURCE SPECTRUM = 2

ALPHA 1 ENERGY = 4.7800 MEV FREQUENCY = 0.9500

ALPHA 2 ENERGY = 4.6000 MEV FREQUENCY = 0.0500

WEIGHTED ENERGY/ALPHA = 4.7710 MEV

NUMBER OF ALPHA PARTICLES USED IN THIS CALCULATION = 10000

NUMBER OF SLABS = 54

ABSORBED DOSE RATE, DOSE EQUIVALENT RATE, AND
DOSE-WEIGHTED LET AS FUNCTIONS OF DEPTH (HISTOGRAM)

SLAB NUMBER	DEPTH (MICRONS)			DOSE RATE (GY/MIN)/(BQ/CM2)	DOSE EQUIVALENT RATE (SV/MIN)/(BQ/CM2)	AVERAGE LET (KEV/MICRON)
1	-6.0518	-	-6.0000	7.4942D-06	1.4988D-04	4.9821D+02
2	-6.0000	-	0.0000	1.2779D-05	2.4009D-04	1.5897D+02
3	0.0000	-	1.0000	9.4609D-06	1.6693D-04	1.4635D+02
4	1.0000	-	2.0000	8.9106D-06	1.5845D-04	1.4903D+02
5	2.0000	-	3.0000	8.3813D-06	1.5025D-04	1.5179D+02
6	3.0000	-	4.0000	7.8982D-06	1.4276D-04	1.5459D+02
7	4.0000	-	5.0000	7.4538D-06	1.3585D-04	1.5741D+02
8	5.0000	-	6.0000	7.0200D-06	1.2890D-04	1.6011D+02
9	6.0000	-	7.0000	6.6060D-06	1.2215D-04	1.6278D+02
10	7.0000	-	8.0000	6.2195D-06	1.1584D-04	1.6558D+02
11	8.0000	-	9.0000	5.8569D-06	1.0992D-04	1.6852D+02
12	9.0000	-	10.0000	5.5027D-06	1.0401D-04	1.7145D+02
13	10.0000	-	11.0000	5.1535D-06	9.8038D-05	1.7435D+02
14	11.0000	-	12.0000	4.8130D-06	9.2125D-05	1.7730D+02
15	12.0000	-	13.0000	4.4809D-06	8.6274D-05	1.8033D+02
16	13.0000	-	14.0000	4.1498D-06	8.0296D-05	1.8331D+02
17	14.0000	-	15.0000	3.8239D-06	7.4315D-05	1.8635D+02
18	15.0000	-	16.0000	3.4949D-06	6.8103D-05	1.8922D+02
19	16.0000	-	17.0000	3.1673D-06	6.1796D-05	1.9201D+02
20	17.0000	-	18.0000	2.8376D-06	5.5303D-05	1.9455D+02
21	18.0000	-	19.0000	2.5009D-06	4.8573D-05	1.9639D+02
22	19.0000	-	20.0000	2.1579D-06	4.1715D-05	1.9716D+02
23	20.0000	-	21.0000	1.8078D-06	3.4714D-05	1.9606D+02
24	21.0000	-	22.0000	1.4509D-06	2.7578D-05	1.9162D+02
25	22.0000	-	23.0000	1.0927D-06	2.0416D-05	1.8152D+02
26	23.0000	-	24.0000	7.4774D-07	1.3524D-05	1.6286D+02
27	24.0000	-	25.0000	4.4183D-07	7.4417D-06	1.3364D+02
28	25.0000	-	26.0000	2.0606D-07	2.9014D-06	9.5828D+01
29	26.0000	-	27.0000	5.9439D-08	6.1130D-07	5.7282D+01
30	27.0000	-	28.0000	2.3774D-09	1.7087D-08	3.5000D+01
31	28.0000	-	29.0000	0.0000D+00	0.0000D+00	0.0000D+00
32	29.0000	-	30.0000	0.0000D+00	0.0000D+00	0.0000D+00
33	30.0000	-	31.0000	0.0000D+00	0.0000D+00	0.0000D+00
34	31.0000	-	32.0000	0.0000D+00	0.0000D+00	0.0000D+00
35	32.0000	-	33.0000	0.0000D+00	0.0000D+00	0.0000D+00
36	33.0000	-	34.0000	0.0000D+00	0.0000D+00	0.0000D+00
37	34.0000	-	35.0000	0.0000D+00	0.0000D+00	0.0000D+00
38	35.0000	-	36.0000	0.0000D+00	0.0000D+00	0.0000D+00
39	36.0000	-	37.0000	0.0000D+00	0.0000D+00	0.0000D+00
40	37.0000	-	38.0000	0.0000D+00	0.0000D+00	0.0000D+00
41	38.0000	-	39.0000	0.0000D+00	0.0000D+00	0.0000D+00
42	39.0000	-	40.0000	0.0000D+00	0.0000D+00	0.0000D+00
43	40.0000	-	41.0000	0.0000D+00	0.0000D+00	0.0000D+00
44	41.0000	-	42.0000	0.0000D+00	0.0000D+00	0.0000D+00
45	42.0000	-	43.0000	0.0000D+00	0.0000D+00	0.0000D+00
46	43.0000	-	44.0000	0.0000D+00	0.0000D+00	0.0000D+00
47	44.0000	-	45.0000	0.0000D+00	0.0000D+00	0.0000D+00
48	45.0000	-	46.0000	0.0000D+00	0.0000D+00	0.0000D+00
49	46.0000	-	47.0000	0.0000D+00	0.0000D+00	0.0000D+00
50	47.0000	-	48.0000	0.0000D+00	0.0000D+00	0.0000D+00
51	48.0000	-	49.0000	0.0000D+00	0.0000D+00	0.0000D+00
52	49.0000	-	50.0000	0.0000D+00	0.0000D+00	0.0000D+00
53	50.0000	-	100.0000	0.0000D+00	0.0000D+00	0.0000D+00
54	100.0000	-	1000.0000	0.0000D+00	0.0000D+00	0.0000D+00

Table 3 (cont.)

ENERGY DEPOSITED/ALPHA IN TOTAL SYSTEM (ALL SLABS) = 4.7710 MEV

ENERGY DEPOSITED/ALPHA IN WATER (SLABS 3 TO 54) = 2.4104 MEV

AVERAGE LET IN WATER (SLABS 3 TO 54) = 167.2007 KEV/MICRON

AVERAGE QUALITY FACTOR IN WATER (SLABS 3 TO 54) = 18.5723

ABSORBED DOSE RATE, DOSE EQUIVALENT RATE, AND
DOSE-WEIGHTED LET AS FUNCTIONS OF DEPTH (GRAPH)

SLAB NUMBER	DEPTH (MICRONS)	DOSE RATE (GY/MIN)/(BQ/CM2)	DOSE EQUIVALENT RATE (SV/MIN)/(BQ/CM2)	AVERAGE LET (KEV/MICRON)
1	-6.0259	7.4942D-06	1.4988D-04	4.9821D+02
2	-3.0000	1.2779D-05	2.4009D-04	1.5897D+02
3	0.5000	9.4609D-06	1.6693D-04	1.4635D+02
4	1.5000	8.9106D-06	1.5845D-04	1.4903D+02
5	2.5000	8.3813D-06	1.5025D-04	1.5179D+02
6	3.5000	7.8982D-06	1.4276D-04	1.5459D+02
7	4.5000	7.4538D-06	1.3585D-04	1.5741D+02
8	5.5000	7.0200D-06	1.2890D-04	1.6011D+02
9	6.5000	6.6060D-06	1.2215D-04	1.6278D+02
10	7.5000	6.2195D-06	1.1584D-04	1.6558D+02
11	8.5000	5.8569D-06	1.0992D-04	1.6852D+02
12	9.5000	5.5027D-06	1.0401D-04	1.7145D+02
13	10.5000	5.1535D-06	9.8038D-05	1.7435D+02
14	11.5000	4.8130D-06	9.2125D-05	1.7730D+02
15	12.5000	4.4809D-06	8.6274D-05	1.8033D+02
16	13.5000	4.1498D-06	8.0296D-05	1.8331D+02
17	14.5000	3.8239D-06	7.4315D-05	1.8635D+02
18	15.5000	3.4949D-06	6.8103D-05	1.8922D+02
19	16.5000	3.1673D-06	6.1796D-05	1.9201D+02
20	17.5000	2.8376D-06	5.5303D-05	1.9455D+02
21	18.5000	2.5009D-06	4.8573D-05	1.9639D+02
22	19.5000	2.1579D-06	4.1715D-05	1.9716D+02
23	20.5000	1.8078D-06	3.4714D-05	1.9606D+02
24	21.5000	1.4509D-06	2.7578D-05	1.9162D+02
25	22.5000	1.0927D-06	2.0416D-05	1.8152D+02
26	23.5000	7.4774D-07	1.3524D-05	1.6286D+02
27	24.5000	4.4183D-07	7.4417D-06	1.3364D+02
28	25.5000	2.0606D-07	2.9014D-06	9.5828D+01
29	26.5000	5.9439D-08	6.1130D-07	5.7282D+01
30	27.5000	2.3774D-09	1.7087D-08	3.5000D+01
31	28.5000	0.0000D+00	0.0000D+00	0.0000D+00
32	29.5000	0.0000D+00	0.0000D+00	0.0000D+00
33	30.5000	0.0000D+00	0.0000D+00	0.0000D+00
34	31.5000	0.0000D+00	0.0000D+00	0.0000D+00
35	32.5000	0.0000D+00	0.0000D+00	0.0000D+00
36	33.5000	0.0000D+00	0.0000D+00	0.0000D+00
37	34.5000	0.0000D+00	0.0000D+00	0.0000D+00
38	35.5000	0.0000D+00	0.0000D+00	0.0000D+00
39	36.5000	0.0000D+00	0.0000D+00	0.0000D+00
40	37.5000	0.0000D+00	0.0000D+00	0.0000D+00
41	38.5000	0.0000D+00	0.0000D+00	0.0000D+00
42	39.5000	0.0000D+00	0.0000D+00	0.0000D+00
43	40.5000	0.0000D+00	0.0000D+00	0.0000D+00
44	41.5000	0.0000D+00	0.0000D+00	0.0000D+00
45	42.5000	0.0000D+00	0.0000D+00	0.0000D+00
46	43.5000	0.0000D+00	0.0000D+00	0.0000D+00
47	44.5000	0.0000D+00	0.0000D+00	0.0000D+00
48	45.5000	0.0000D+00	0.0000D+00	0.0000D+00
49	46.5000	0.0000D+00	0.0000D+00	0.0000D+00
50	47.5000	0.0000D+00	0.0000D+00	0.0000D+00
51	48.5000	0.0000D+00	0.0000D+00	0.0000D+00
52	49.5000	0.0000D+00	0.0000D+00	0.0000D+00
53	75.0000	0.0000D+00	0.0000D+00	0.0000D+00
54	550.0000	0.0000D+00	0.0000D+00	0.0000D+00

TIME = 2.3348 MINUTES

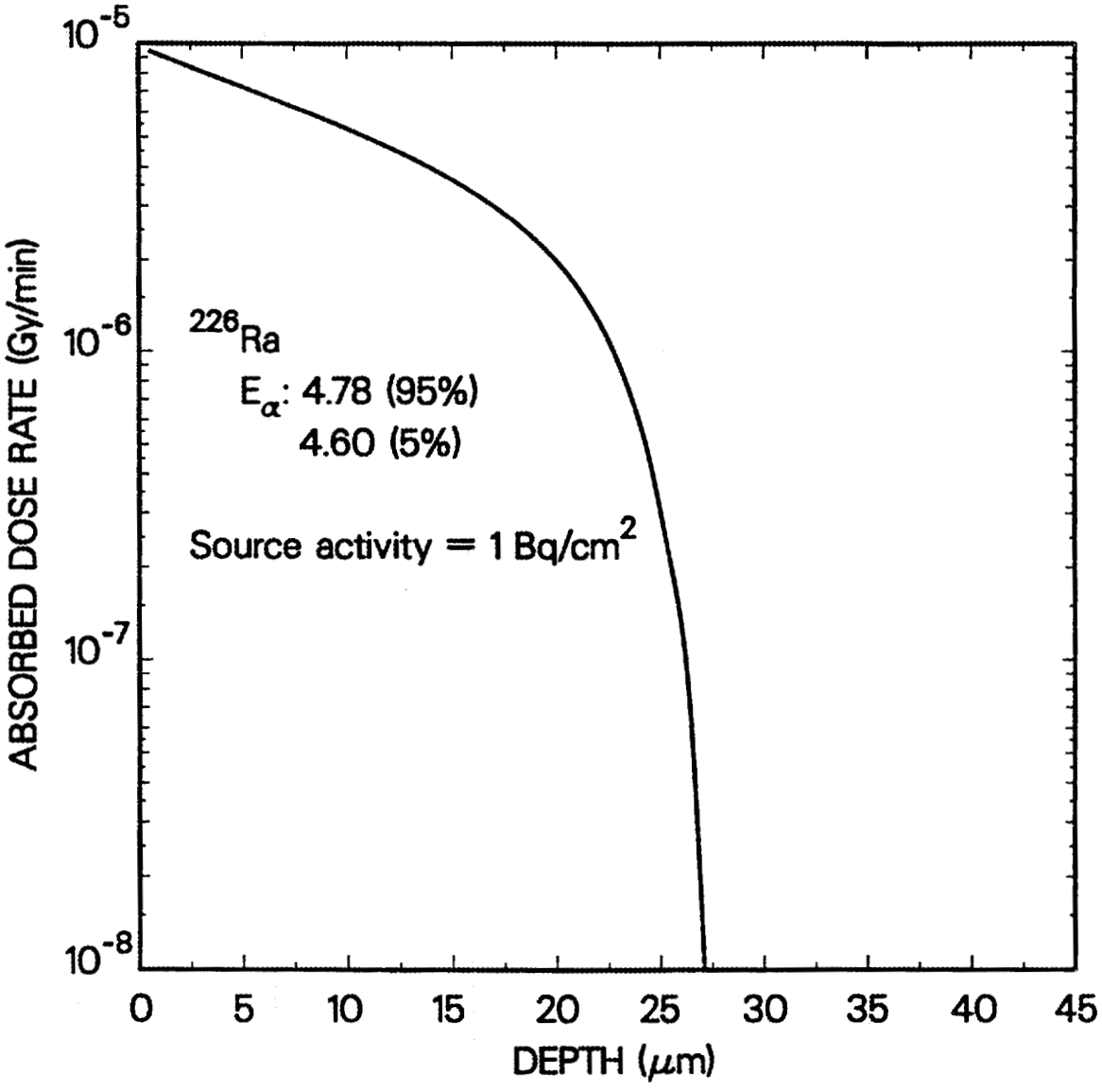

Fig. 3 Absorbed-dose rate (Gy/min) as a function of depth for a ^{226}Ra disc source (1 Bq/cm^2) separated from water target (starting at Z=0) by 0.0518 μm of gold and 6.000 μm of Mylar.

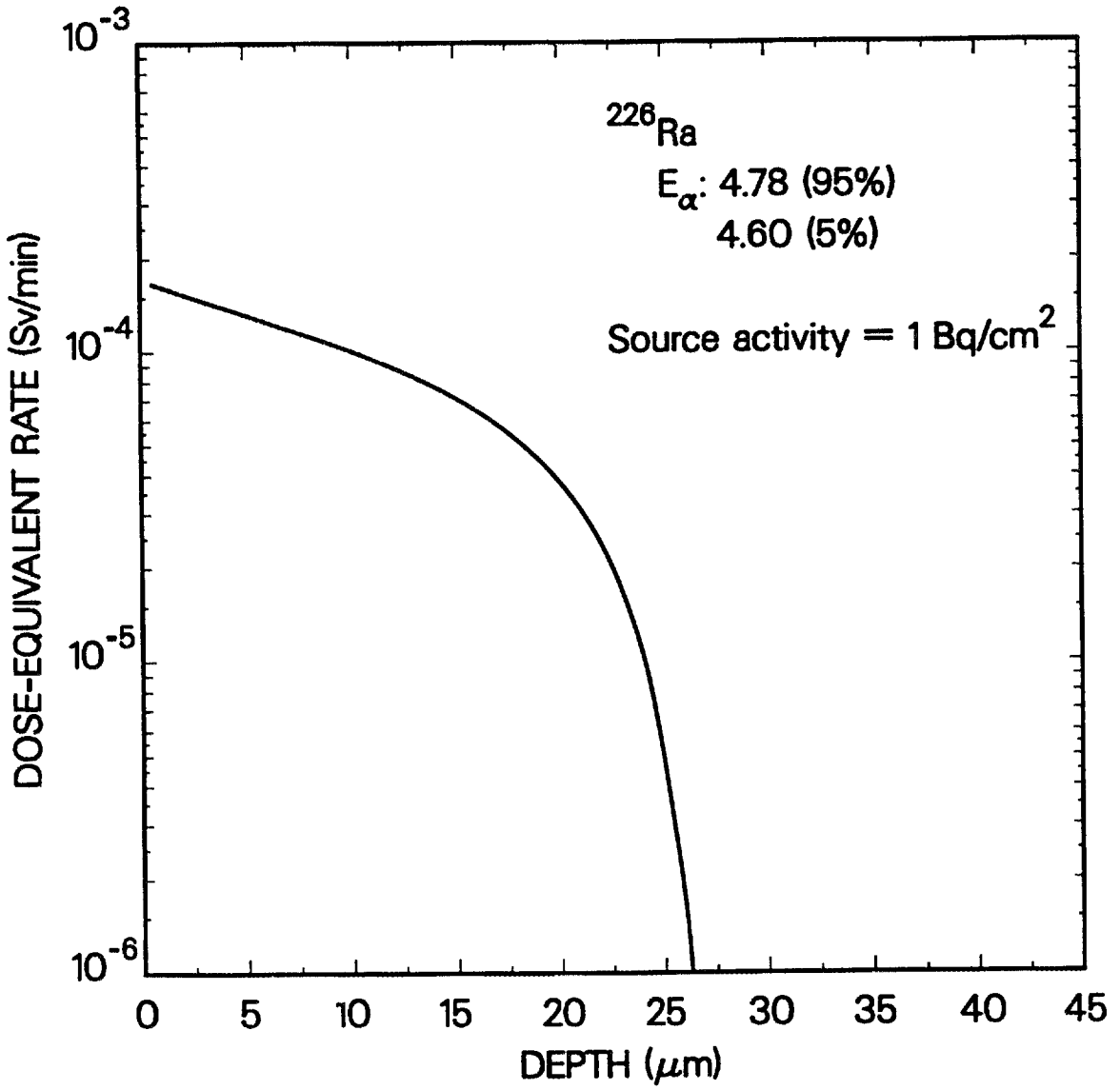

Fig. 4 Dose-equivalent rate (Sv/min) as a function of depth in water for ^{226}Ra source with same geometry as Fig. 3. The average quality factor is 18.6.

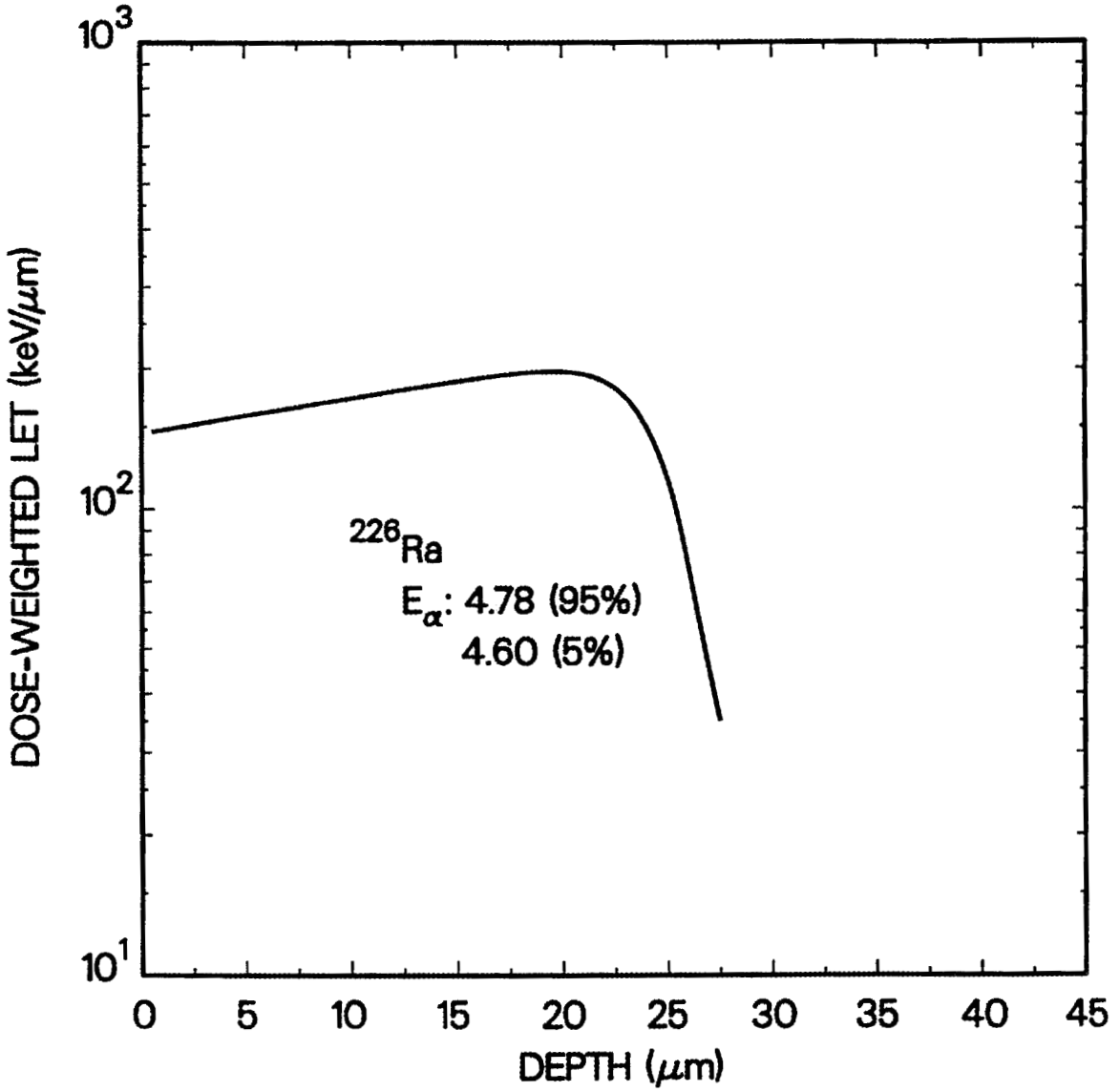

Fig. 5 Dose-weighted LET (keV/μm) as a function of depth in water for ^{226}Ra source with same geometry as Fig. 3. The average LET over all irradiated water is 167 keV/μm.

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