A Method for Calculating Single-Event Distributions for Point Source Alpha Emitters

by
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A METHOD FOR CALCULATING SINGLE-EVENT
DISTRIBUTIONS FOR POINT SOURCE
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ABSTRACT

A method is described for calculating single-event distributions for point source alpha emitters. The method is based on computer simulation of alpha particle track structure by Monte Carlo techniques.

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A METHOD FOR CALCULATING SINGLE-EVENT DISTRIBUTIONS FOR POINT SOURCE ALPHA EMITTERS*

W. E. Wilson

INTRODUCTION

The theoretical nature of the distributions of energy deposited in microscopic volumes of matter by radiation fields have been extensively discussed by Kellerer¹ and by Roesch and Glass.² Experimental measurements have been reported by Glass and Braby,³ Gross, et al.,⁴ and Glass and Roesch.⁵ For a general review, see Rossi.⁶

It is the purpose of this note to describe a method for calculating the single-event distribution in energy imparted^a for a point source alpha emitter. The need for these distributions arises as a practical matter in the microdosimetry of internal emitters.⁷

FORMALISM

The single-event distribution in energy imparted for a point source at a distance r_0 from a spherical volume of radius ρ is (see Fig. 1),

$$F_1(e) = \int_{\Omega} n(\Omega) f_1(e, \vec{r}) d\Omega \quad (1)$$

where $n(\Omega)$ is the flux density, and $f_1(e, \vec{r})$ is the energy imparted

*This paper is based on work performed under United States Energy Research and Development Agency Contract EY-76-C-06-1830.

^aSee ICRU-19 for definitions.

by a single track at $\vec{r}$ in the volume of interest. The volume of integration must extend over all solid angles for which f_1 is non-zero. Because of the finite range of the most energetic δ -rays, this volume is slightly larger than the site volume. For an isotropic source of activity, N,

$$n(\Omega) = \frac{N}{4\pi},$$

$$\text{also } d\Omega = \sin\theta \, d\theta \, d\phi.$$

Because the problem has rotational symmetry, f_1 does not depend on ϕ , therefore, Eq.(1) can be written

$$F_1(e) = \frac{N}{2} \int_0^\pi \sin\theta \, f_1(e, r, \theta) \, d\theta \quad (2)$$

And, because of the rotational symmetry, the $f_1(e, r, \theta)$ can be completely characterized by $f_1(e, a)$, that is, all f_1 's having the same impact parameter, a , are identical.

DETERMINATION OF $f_1(e, a)$ FOR $a < \rho$

Monte Carlo techniques were used to evaluate $f_1(e, a)$ for $a < \rho$ and for the range of alpha particle energies 1-6 MeV and sites of radii 0.1-5.0 micrometers. The calculations were made using computer codes developed by Paretzke.⁸ Typical results are shown in Fig. 2 for 6 MeV alphas passing at various impact parameters through a site radius .25 μm . The distributions are only very roughly bell shaped because of low statistical accuracy in the calculations but are qualitatively in agreement with

experimental measurements by Glass and Roesch.⁵ No quantitative comparison was made because their experimental work was done with protons passing through a cylindrical site of tissue-equivalent gas.

We have approximated the distributions by a Gaussian function of the form,

$$f_1(e, a) = \frac{1}{\sqrt{2\pi}\sigma(a)} \text{EXP} \left(-\frac{1}{2} \left(\frac{e - \bar{\Delta}(a)}{\sigma(a)} \right)^2 \right) \quad (3)$$

where $\bar{\Delta}(a)$ is the centroid or mean and $\sigma(a)$ is the standard deviation or width of the distribution.

The dependence of $\bar{\Delta}$ and of σ on the impact parameter, a , obtained from the Monte Carlo calculations is shown in Fig. 3. The shape of the curve for $\bar{\Delta}$ indicates that it is linearly related to the track length inside the site (x in Fig. 1). This is to be expected because for the energies and site sizes considered here, the energy imparted to the site should nearly equal the energy lost by the alpha particle in passing through the site. That is,

$$\bar{\Delta}(a) = L \cdot x(a) \quad (4)$$

where L is the LET (stopping power) of the medium.

The dependence of the width of the distribution on radial position is also shown in Fig. 3. The ratio, $\sigma/\bar{\Delta}$, is constant out to within $0.1 \mu\text{m}$ of the edge of the site, then it increases sharply. This sharp increase has been approximated by ^{an}exponential. Therefore, the width of the Gaussian distribution is given by

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$$\sigma(a)/\Delta(a) = 0.12, \text{ for } 0 < a < \rho - 0.1, \quad (5)$$

$$\text{and } \sigma(a)/\Delta(a) = 0.12 + 0.45 \exp(-107(r-a)), \text{ for } \rho - 0.1 < a < \rho. \quad (6)$$

Numerical integration of Eq.(2) using equations 3-6 is sufficient to evaluate single-event distributions for tracks which pass through the site.

EFFECT OF TRACKS WITH $a > \rho$

The contribution to F_1 (Eq.(2)) for tracks passing outside the site is estimated entirely from Monte Carlo calculations and in the uniform flux or distant source approximation. Consider equations 1 and 2 and Fig. 1, for large r_0 , we have

$$\sin \theta \approx \theta \approx a/r_0, \text{ and } d\theta = da/r_0. \quad (7)$$

Therefore, in this approximation, the contribution, $F'_1(e)$, for tracks passing outside the site is

$$F'_1(e) = \frac{N}{4\pi r_0^2} 2\pi \int_{\rho}^{\infty} a f_1(e, a) da \quad (8)$$

For numerical evaluation, the continuous integral can be approximated by a finite sum. Taking all a_i of equal size and letting $g = 4\pi r_0^2 F'_1/N$, then,

$$g(e) = 2\pi \Delta a \sum_i a_i f_1(e, a_i), \quad (9)$$

$f_1(e, a_i)$ goes to zero rapidly for increasing $a_i > \rho$. Therefore, only a few terms with $a_i \sim \rho$ need to be considered in Eq.(9).

Because of this feature, $g'(e, E_\alpha, a) = g(e)/\rho$ should be relatively independent of site size, ρ .

Single-event distributions, g' , were calculated for track 5 with $\rho < a < (\rho + .3)\mu\text{m}$ for alpha energies over the range $1 < E_\alpha < 6$ MeV and for $0.1 < \rho < 5\mu\text{m}$. A summary of the results is shown in Fig. 4. The single-event distribution for tracks which pass totally outside the site is not significantly dependent on alpha energy and can be adequately approximated with an algorithm exponential in energy imparted, e . The amplitude and characteristic decay are, as expected, not strong functions of ρ ; only the decay is assumed to vary linearly with site radius. Hence,

$$g'(e, a) = A \text{ Exp } (be) \quad (11)$$

$$\text{where } A = 0.12, \text{ and} \quad (12)$$

$$b = -0.92 + 0.175\rho, \text{ from least-square-fitting of Eq.(11) to the data presented in Fig. 4.}$$

Then,

$$F'_1(e) = \frac{N}{4\pi r_o^2} A \text{ Exp } (be) \quad (14)$$

APPENDIX

A. Description

Subroutine SINGLE (see Appendix B for listings) does a numerical integration of Eq.(2) over the volume of the site using equations 3-6, and adds Eq.(14) at the end to represent the effect

of tracks which pass outside the site. The LET needed for Eq.(4) is evaluated from Brice's semi-empirical formulation for stopping power.⁹ The LET for water is obtained from Bragg's rule and Brice's parameters for helium atoms in hydrogen and in oxygen and is calculated by the two function subprograms RLET(EA) and S(EALPH,I).

This version of SINGLE returns single-event distributions for different values of r_0 (Fig. 1) beginning with $r_0 = 0$, and increasing in $1\mu\text{m}$ steps until the range of the alpha is reached, up to a maximum of 40 steps. (The range of a 5.15 MeV alpha is about $39\mu\text{m}$ in homogeneous tissue or H_2O .)

Definitions

All subroutine input-output for SINGLE is passed via COMMON. CMI (input)-EA is alpha particle energy in MeV, RO is site radius in micrometers, N is a dimension parameter for the output arrays. CMO (output)-F(I,J), $1 \leq I \leq N$ is the calculated result for the Jth r_0 ($r_0(1) = 0$). E(I,J) is the energy scale in keV for F(I,J). RE(J) is the residual alpha energy in MeV at the center of the site for the Jth value of r_0 . It is calculated in a continuous slowing down approximation using Brice's formulation for stopping power and taking discrete steps of not larger than 50 keV energy loss. RANG is the total distance covered in the above approximation when the residual alpha energy decreases to less than 10 keV. KMAX is the actual number of cases or distributions to be calculated; it is the range +1 in integer μm .

AVG(50), SIG(50) and B(50) are scratch arrays.

Method

The array RE is calculated between lines 11 and 29. (Unless otherwise specifically stated, references to the listing will be by line number rather than by statement number). The site radius is restricted to be larger than $0.1\mu\text{m}$ at 11, other initial assignments are made at lines 13 and 14. The basic loop for calculating an RE is from line 15 to 27, with an exit at line 23 if the residual energy becomes less than 10 keV. An integer distance in μm is assigned at 17, a current value of stopping power (LET) in $\text{keV}/\mu\text{m}$ is obtained at 18. A decremental energy step is assigned at 20. The code iterates between 18 and 24 taking no more than 50 keV energy-loss steps until a distance is accumulated equal to that assigned at 17. When that happens RE(k) is assigned at 25, KMAX is updated to K. Upon eventual exit at line 23, KMAX will equal the last valid K.

At 29, RANG is assigned to be the total distance accumulated. The evaluation of the KMAX single-event distributions is accomplished by the DO loop between lines 30 and 83. Initialization takes place between 31 and 39. The energy scale is determined at line 38, based on LET, site size and number of channels in the arrays. The energy array is assigned and the distribution array cleared between lines 40 and 43.

Equation 2 is evaluated in two steps, the first step extends from lines 44 to 60, the second from 61 to 78. The first step does

the integral in polar coordinates in 50 equal intervals in θ for $0 < a < (\rho - .1)$. The second completes the integration, that is for $(\rho - .1) < a < \rho$ also in 50 equal intervals (the size of the latter intervals is generally much smaller than the former). This procedure is used in order to avoid artifacts in the calculated distributions arising from the numerical method. A very fine integration grid is required for tracks near the edge of the site. In the first step, equations 4 and 5 are evaluated at lines 54 and 55 and in the second step equations 4 and 6 are evaluated between 69 and 73. The actual integration (summation) is done at line 60 and at line 78.

$F'_1(e)$ (Eq.14) is evaluated by the function subprogram SEP(Y,R) and is added to the previous result at line 81.

Figure 1

Schematic representation of the problem. A point alpha source emits $n(\Omega)$ alpha's per steradian. A typical alpha makes a track of length x as it passes through the absorber site of radius ρ at a distance r_0 from the emitter. In the text, the distance, a , is called an impact parameter.

Figure 2

Energy deposition distributions for individual 6 MeV alpha particles passing at different impact parameters through a site of $.25 \mu\text{m}$ radius.

Figure 3

Dependence of the mean, $\bar{\Delta}$, and width, σ , of energy deposition distributions on impact parameter for individual tracks passing through the absorber site.

Figure 4

Energy deposition distributions (divided by site radius) in energy imparted for 3 and 6 MeV alphas passing totally outside sites of radius 0.5 and 2.5 μm .

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APPENDIX A


```

1      SUBROUTINE SINGLE
CC-    THIS VERSION CALCULATES PROBILITY DENSITY IN ENERGY IMPARTED
CC-    FROM A POINT SOURCE, AUTH-WE WILSON, RICHLAND WA99352 (4/12/77)
      COMMON /CHI/EA,RO,N
5      COMMON /CMO/E(128,40),F(128,40),RE(40),RANG,KMAX
      DIMENSION AVG(50),SIG(50),B(50)
      REAL L
      DATA AVG/50*0.,/,SIG/50*0.,/,B/50*0./
      DATA C1/,1994711/,PI/3,141592654/
10     FEXP(Z)=EXP(AMAX1(-293.,AMIN1(321.,Z)))
      R=AMAX1(RO,.10001)
CC-    GET RESIDUAL ENERGY AT 1. MICRON INTERVALS
      REA=EA
      X=0.
15     DO 10 K=1,40
          RE(K)=0.
          XK=FLOAT(K-1)
          5      L=RLET(REA)
          Y=L*AMAX1(1,E-14,(XK-X))
          DE=AMIN1(Y,AMAX1(50.,50.*REA))
          X=X+DE/L
          REA=REA-.001*DE
          IF(REA,LE.,.010) GO TO 15
          IF(X,LT.,XK) GO TO 5
25     RE(K)=REA
          KMAX=K
          10     CONTINUE
CC-    LAST VALUE IS 'RANGE'
          15     RANG=X
30     DO 90 K=1,KMAX
          REA=RE(K)
          IF(REA,LE.,.010) GO TO 90
          RNG=FLOAT(K-1)
          C2=4.*PI*RNG**2
          35     L=RLET(REA)
CC-    SET UP ENERGY SCALE AND CLEAR FUNCTION ARRAY
          IF(N,LE,0) RETURN
          DE=2.7*L*R/FLOAT(N)
          Y=0.
40     DO 20 J=1,N
          F(J,K)=0.
          Y=Y+DE
          20     E(J,K)=Y
CC-    DO INTEGRAL UP TO R=.1
          TH1=PI
          IF(RNG,GE,R) TH1=ASIN((R-.1)/RNG)
          DTH=.02*TH1
          TH=-DTH/2.
          DO 30 I=1,50

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50      TH=TH+DTH
      B(I)=SIN(TH)
      X      =2.*SQRT(R**2-(RNG*B(I))**2)
      IF(RNG.LT,R)X=RNG*SQRT(1,-B(I)**2)+X/2,
      AVG(I)=AMIN1(L*X,REA*1.E3)
55      SIG(I)=.12*AVG(I)
      B(I)=B(I)*DTH*C1/SIG(I)
      30  CONTINUE
      DO 40 J=1,N
      DO 40 I=1,50
60      40  F(J,K)=F(J,K)+B(I)*FEXP(-.5*((E(J,K)-AVG(I))/SIG(I))**2)
      IF(RNG.LT,R) GO TO 90
CC-     DO INTEGRAL ON OUT TO R
      TH2=  ASIN(R/RNG)
      DTH=.02*(TH2-TH1)
65      TH=TH1+.5*DTH
      DO 50 I=1,50
      TH=TH+DTH
      B(I)=SIN(TH)
      AVG(I)=L*2.*SQRT(R**2-(RNG*B(I))**2)
70      Y=-107.*(R-(RNG*B(I)))
      Y=AMIN1(Y,0,)
      X=.12+.45*FEXP(Y)
      SIG(I)=X*AVG(I)
      B(I)=B(I)*DTH*C1/SIG(I)
75      50  CONTINUE
      DO 70 J=1,N
      DO 60 I=1,50
60      F(J,K)=F(J,K)+B(I)*FEXP(-.5*((E(J,K)-AVG(I))/SIG(I))**2)
CC-     ADD THE OUTSIDE TRACKS
80      X=E(J,K)
      F(J,K)=F(J,K) +SEP(X,R)/C2
      70  CONTINUE
      90  CONTINUE
      IER=0
85      RETURN
      END

```


APPENDIX B


```

1      FUNCTION SEP(Y,R)
      CC= THIS FUNCTION RETURNS THE PROBABILITY DENSITY IN Y
      CC= FOR TRACKS WHICH PASS OUTSIDE THE SITE
      C   Y=ENERGY IMPARTED IN KEV
5      C   R=SITE RADIUS IN MICROMETERS
      C   SEP IS RETURNED IN UNITS OF KEV**-1
      C
      B=.175*R-.92
      B=AMIN1(0.,B)
10     C
      SEP=0.12*EXP(B*Y)*R
      RETURN
      END

1      FUNCTION RLET(EA)
      C   THIS FUNCTION GETS LET FOR ALPHAS IN H2O FROM BRAGS RULE AND BRICE
      C   LET IS RETURNED IN UNITS OF KEV/MICROMETER,
5      S1=10.*S(EA,1)
      S2=6.*S(EA,2)
      RLET=3.35E15*(S1+S2)
      RETURN
      END

1      FUNCTION S(EALPH,I)
      C   THIS FUNCTION RETURNS THE STOPPING CROSS SECTION FOR ALPHAS
      C   OF ENERGY EA(MEV) IN OXYGEN (I=1) OR HYDROGEN (I=2).
      C   REF= D.K.BRICE,PHYS.REV,A6,1794(1972),
5      C   RETURNED QUANTITY IS IN EV*CM**2/ELECTRON
      DIMENSION A(2),N(2),Z(2)
      REAL N
      DATA A/,3866,,4441/,N/3.49,3.668/,Z/1.3402,1.1812/
      EA=AMAX1(EALPH,.001)
10     UOC=SQRT(5.3657E-4*EA)
      ERT=68.5*UOC/Z(I)
      E1=ERT*ERT
      E2=E1*E1
      E3=E2*E1
15     FU=1./((1.+(137.*A(I)*UOC)**N(I))
      SPU=ERT*(30.*E3+83.*E2+74.*E1+21.)/(3.*(1.+E1)**3)+
1     (10.*E1+1.)*ATAN(ERT)
      S=.609E-15*SPU*FU
      RETURN
20     END

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