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Robert Katz

*University of Nebraska-Lincoln*, rkatz2@unl.edu

Kim Sum Loh

*University of Nebraska-Lincoln*

Luo Baling

*University of Nebraska-Lincoln*

Guo-Rong Huang

*University of Nebraska-Lincoln*

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# An Analytic Representation of the Radial Distribution of Dose from Energetic Heavy Ions in Water, Si, LiF, NaI, and SiO<sub>2</sub>

Robert Katz, Kim Sum Loh, Luo Baling, and Guo-Rong Huang

University of Nebraska–Lincoln, Lincoln, NE 68588-0150

## Abstract

An earlier representation of the radial distribution of dose about the path of a heavy ion in liquid water is modified and extended to include silicon, lithium fluoride, sodium iodide, and silicon dioxide.

**Keywords:** Dose distribution, heavy ion, heavy ion track, track registration, radiation effects, stopping power, silicon, silicon dioxide, lithium fluoride, sodium iodide

## Introduction

We seek to simplify a set of equations recently developed to describe the radial distribution of dose from energetic heavy ions in liquid water<sup>1</sup> and to alter them systematically to yield an approximation to the radial distribution of dose in other substances, subject to the only available constraint, namely that the resulting formulation should, on radial integration, yield the stopping power for protons. Our results for the dose distribution for heavy ions in silicon are in reasonable agreement with the results of an earlier Monte Carlo calculation.<sup>2</sup>

## Dose in Water

We show in Figure 1 a set of equations for the calculation of the radial dose distribution in liquid water from energetic ions, from our earlier work, based on a Monte Carlo calculation of the dose distribution from protons in liquid water.<sup>1</sup> Here the quantity represented by  $D_1$ , Equation (1), is taken to be the dose deposited by delta rays and the quantity  $D_1K$ , Equation (11), is interpreted as the contribution to the radial dose from primary excitations and ionizations. These sum to the quantity  $D_2$  Equation (11), the total radial dose. These equations have been used to calculate the response of the Fricke dosimeter<sup>3</sup> and the inactivation of dry enzymes and viruses<sup>4</sup> to good effect through use of the track theory of 1-hit detectors.

In the present work we have sought to extend these calculations to other materials, and in so doing have made a simplified representation of the quantity  $K$ , Equation (12), now represented as  $k$  as shown in Equation (18) below.

For energies  $> 0.1$  and  $< 1000$  MeV/amu we now have

$$k(t) = a\beta^b \exp(-t/c), \quad (18)$$

where  $t$  is the radial distance from the ion's path,  $\beta$  is the speed of the ion relative to the speed of light, and  $a$ ,  $b$ , and  $c$  are adjustable constants. In order to make the present

Radial dose distribution:

$$D_1(t) = \frac{Ne^4 Z^{*2}}{\alpha mc^2 \beta^2 t} \cdot \frac{(1 - ((t+\theta)/(T+\theta)))^{1/\alpha}}{t+\theta} \quad (1)$$

$$\theta = R(I) \quad I = 10 \text{ eV} \quad (2)$$

$$T = R(W) \quad W = 2mc^2 \beta^2 (1-\beta^2)^{-1/2} \quad (3)$$

Electron range-energy relation for aluminium:

$$R = k \cdot w^\alpha \quad (4)$$

$$k = 6 \times 10^{-6} \text{ g} \cdot \text{cm}^2 \cdot \text{keV}^{-\alpha} \quad (5)$$

$$w < 1 \text{ keV} \quad \alpha = 1.079 \quad \text{for ion} \quad \beta \leq 0.03 \quad (6)$$

$$w > 1 \text{ keV} \quad \alpha = 1.667 \quad \text{for ion} \quad \beta > 0.03 \quad (7)$$

Delta ray distribution:

$$dn = \frac{2\pi Ne^4 Z^{*2}}{mc^2 \beta^2} \cdot \frac{dw}{(w+I)^2} \quad (8)$$

Constant for liquid water:

$$N = \frac{2\pi Ne^4}{mc^2 \beta^2} = 1.369 \times 10^{-14} \text{ J} \cdot \text{cm}^{-1} = 8.5 \text{ keV} \cdot \text{mm}^{-1} \quad (9)$$

Effective charge:

$$Z^* = Z(1 - \exp(-125 \cdot \beta \cdot Z^{-2/3})) \quad (10)$$

Corrected radial dose distribution:

$$D_2(t) = D_1(t) \cdot (1 + K(t)) \quad (11)$$

$$K(t) = A \cdot ((t-B)/C) \cdot \exp(-(t-B)/C) \quad (12)$$

$$A = 8 \cdot \beta^{1/3} \quad \text{for} \quad \beta \leq 0.03 \quad (13)$$

$$A = 19 \cdot \beta^{1/3} \quad \text{for} \quad \beta > 0.03 \quad (14)$$

$$B = 0.1 \text{ nm} \quad (15)$$

$$C = 1.5 \text{ nm} + \beta \cdot 5 \text{ nm} \quad (16)$$

$$K(t) = 0 \quad \text{for} \quad t < B \quad (17)$$

**Figure 1.** Equations for the radial dose distribution in liquid water, from Waligorski *et al.*<sup>1</sup>

scheme work for a variety of materials we have found it necessary to treat the "effective ionization potential for delta ray production,"  $I$ , Equation (2), as an adjustable parameter as well.

The assigned values of the parameters  $a$ ,  $b$ ,  $c$ , and  $I$  for water and other materials, are given in Table I.

**Table I.** Parameters of the new radial dose distribution functions

Medium	<i>a</i>		<i>b</i>	<i>c</i> (nm)	<i>I</i> (eV)*	<i>G</i> (g/cm <sup>3</sup> )
	low $\beta$	high $\beta^{**}$				
Water	10	23	0.38	4	10	0.56
LiF	6.5	20	0.40	4	10	1.22
Si	2	21	0.54	4	20	1.16
NaI	3	15	0.575	4	40	1.57
SiO <sub>2</sub>	9.3	20	0.42	4	20	1.32

\* *I* is the adjusted ionization potential.

\*\*low  $\beta$  is  $0.01 < \beta < 0.03$ , and high  $\beta$  is  $\beta > 0.03$ .

Other adjustments in our formula for the radial dose distribution to accommodate for variations in electron density, via atomic number, *Z*, mass number, *A*, and density of the medium,  $\rho$ , will be discussed later.

When all of these adjustments are made, the ratio of the radially integrated values of stopping power for protons of different energies lie within 10% of the values given by Janni.<sup>5</sup>

Equation (18) is somewhat simpler in form than that used in our earlier work, Equation (12), and provides an equally good approximation to the Monte Carlo calculation of Hamm for water. The simplification in form makes it somewhat easier to modify for other substances.

We write

$$d_2(t) = d_1(t)(1 + k(t)) \quad (19)$$

and display calculated graphs of the radial dose distributions, both  $D_2$  from the earlier work, Equation (11), and  $d_2$  from the present work, Equation (19), in Figure 2, in comparison with the results of the Monte Carlo calculation.

### Dose in Other Media

We seek to make an empirical approximation to the radial distribution of dose in other materials, of density  $\rho$ , effective atomic number *Z*, and effective mass number *A*. For atomic substances the effective atomic number and mass number are unaltered from those of the atom. For water, LiF, NaI, and SiO<sub>2</sub>, we have taken the effective numbers to represent molecules so that the effective charge and mass number for water are 10 and 18, respectively, while for LiF they are 12 and 26, for NaI they are 64 and 150, and for SiO<sub>2</sub> they are 22 and 44.

We make use of a factor *G* (proportional to the electron density), specific for each medium,

$$G = \rho Z/A \quad (20)$$

to alter both the dose and the radial distance from that in water to that in the new substance *x*, corresponding to the change in the linear density of delta rays and their radial penetration, correcting for the differences in the number density of electrons in the different media.

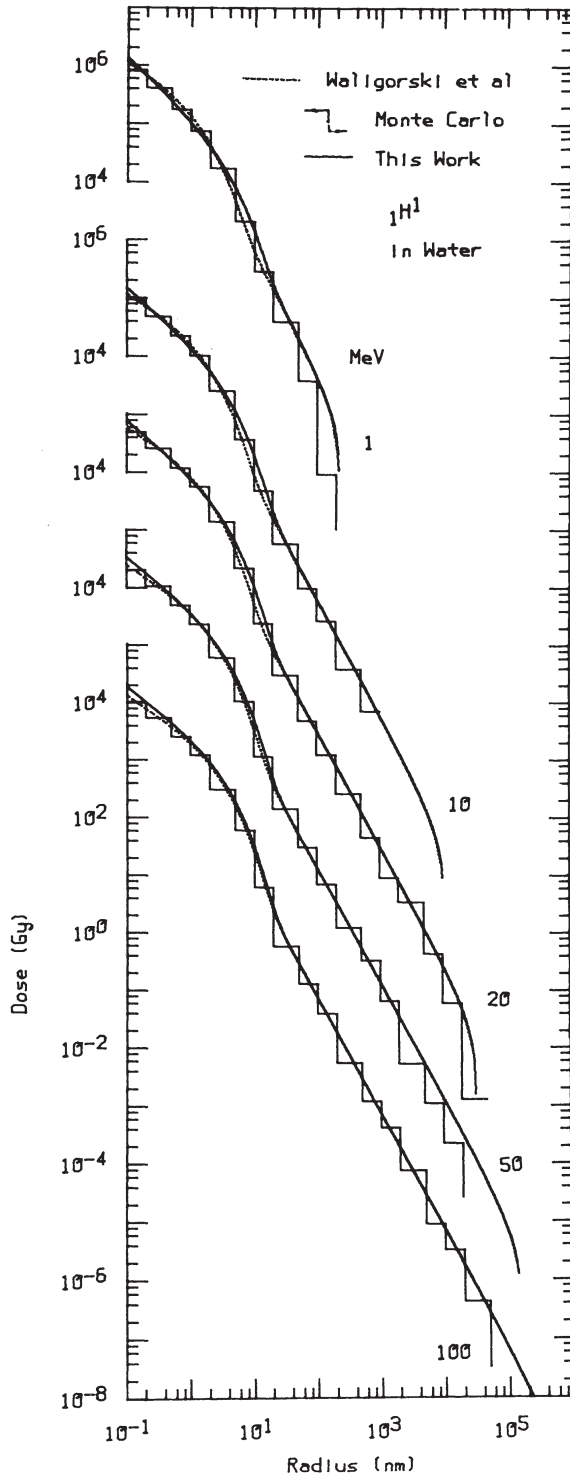


Figure 2. A comparison of the present formulation, that of Waligorski *et al.*, and the Monte Carlo calculation they represent.

We proceed in steps, first recalculating the dose from delta rays by a cubic correction in the ratio of the  $G$  values of the two media to accommodate both the linear density of delta ray production and the effect of electron stopping power on the energy deposited in a cylindrical shell, and second, by a linear correction involving the  $G$  ratios to alter the shell radius in which the energy is deposited, again because of electron stopping power differences in the two media.

We first alter the dose from delta rays  $d_1$  [Equation (1)] in water at radial distance  $t_w$  by use of a factor  $1/G^3$ , as shown in Equation (21), and then reposition that dose from  $t_w$  to  $t_x$  by use of the factor  $G$ , as shown in Equation (22).  $d_{1w}$  is the delta ray dose in water, while the  $d_{1x}$  is the delta ray dose in the medium  $x$ . We write

$$[d_1/G^3]_w = [d_1/G^3]_x \quad (21)$$

The subscript  $w$  on the bracket at left indicates that all quantities in the bracket are for water, and similarly subscript  $x$  on the bracket on right indicates that all quantities in the bracket are in the medium  $x$ .

Not only is the dose different in the two media but also the radial coordinate at which the revised dose is located must be altered. Using similar notation we have

$$[tG]_w = [tG]_x \quad (22)$$

This mapping yields for us the quantity  $d_{1x}$ , the distribution of dose from delta rays at the radial distance  $t_x$  in the new substance  $x$ . Combining Equations (21) and (22), we then display an expression for the dose in  $x$  as a function of the dose in water in Equation(23).

$$d_{1x}(t_x) = (G_x/G_w)^3 d_{1w}(t_x G_x/G_w) \quad (23)$$

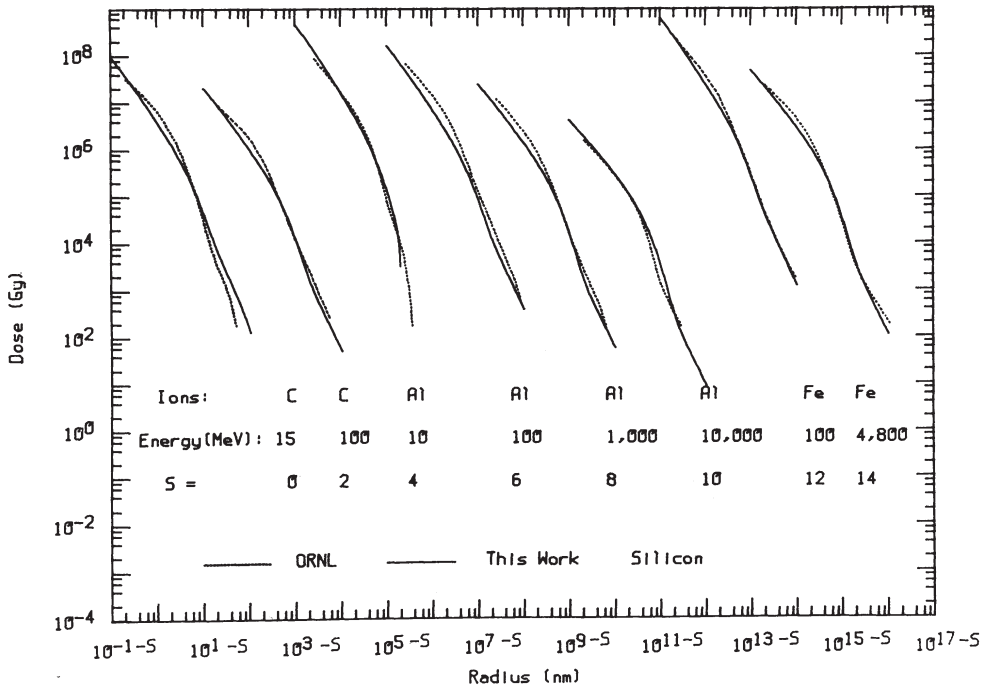
As in Figure 1, we represent the radial dose from delta rays  $d_{1x}$  and the dose from primary interactions  $d_{1x}k_x$  in the medium  $x$  at radial distance  $t_x$  by the expression

$$d_{2x}(t_x) = d_{1x}(t_x)[1 + k_x(t_x)] \quad (24)$$

and now seek to find new numerical values of the parameters  $a$ ,  $b$ ,  $c$ , and  $l$ , as constrained by the requirement that the radial integral of the dose distribution approximates the proton stopping power, as given by the tables of Janni. The values we have found are shown in Table I.

Monte Carlo calculations of the radial dose distribution have been made for Si by Hamm *et al.*<sup>2</sup> In Figure 3 we compare the results of our fitted analytic formula to the result of their Monte Carlo calculations. For different ions we have multiplied our proton calculations by the square of the ratio of the effective charge, Equation (10), of the ion to that for a proton of the same velocity. For silicon it appears that our procedure yields a good analytic approximation to the radial dose distribution obtained by a much more complex, though possibly more accurate, calculation. For the Monte Carlo calculations the comparison between the radial integral of the dose and tabular values of the stopping power has not been given.

Finally, we wish to call attention to recent work by Heckman *et al.*<sup>6</sup> in which the effective charge formula we use is modified to incorporate some recent stopping power mea-



**Figure 3.** The present calculation of the radial dose distribution in Si from C, Al, and Fe ions of different energies to Monte Carlo calculations made at Oak Ridge by Hamm *et al.*<sup>2</sup>

measurements made with Au ions which reflect a variation in the “stopping power effective charge” with the composition of the medium. We have not yet had the opportunity to explore the extent to which this revised effective charge formula will alter our results.

### Acknowledgment

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