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# Energy Deposition Fluctuations Induced by Ions in Microvolumes and Nanovolumes — An Analytic Approach I. Theory

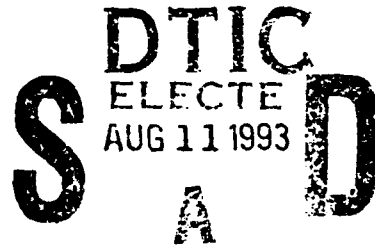
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## NOTATION

$\bar{c}$	average chord length of the site
$D$	total dose deposited in the site
$D_e$	dose deposited in the site by electrons
$D_{ion}$	dose deposited in the site by ions
$d$	dose deposited in the site by one particle
$d_e$	dose deposited in the site by one electron
$d_{ion}$	dose deposited in the site by one ion
$d(y)$	dose weighted probability density function for lineal energy
$d(z)$	dose weighted probability density function for specific energy
$d_1(z)$	dose weighted probability density function for specific energy per event
$E$	total energy deposited in the site
$E_e$	energy deposited in the site by electrons
$E_{ion}$	energy deposited in the site by ions
$F$	Fano factor
$F_e$	Fano factor for electrons
$F_{ion}$	Fano factor for ions
$f_{ion}$	fraction of dose deposited in the site by ions
$1-f_{ion}$	fraction of dose deposited in the site by electrons
$f(N)$	probability density function for number of particle events in the site
$f(x)$	probability density function for number of occurrences of $x$
$f(y)$	frequency weighted probability density function for lineal energy
$f(z)$	frequency weighted probability density function for specific energy
$f_1(z)$	frequency weighted probability density function for specific energy per event
$L$	(unrestricted) Linear Energy Transfer of a particle in the site
$L_e$	(unrestricted) Linear Energy Transfer of an electron in the site
$L_{ion}$	(unrestricted) Linear Energy Transfer of an ion in the site
$N$	number of events in the site
$N'$	fixed value of $N$
$N_A$	number of events in the $A$ -distribution
$N_B$	number of events in the $B$ -distribution
$N_e$	number of electron events in the site
$N_{ion}$	number of ion events in the site
$n$	number of collisions undergone by a particle in the site
$n_e$	number of collisions undergone by an electron in the site
$n_{ion}$	number of collisions undergone by an ion in the site
$P$	normalized or relative frequency of the $A$ -distribution; fraction of events due to ions
$1-P$	normalized or relative frequency of the $B$ -distribution; fraction of events due to electrons
$S_0$	surface area of the site
$s$	path length of a particle in the site
$s_e$	path length of an electron in the site
$s_{ion}$	path length of an ion in the site

$V_D$	relative variance of the total dose deposited in the site
$V_{D,e}$	relative variance of the dose deposited in the site by electrons
$V_{D,ion}$	relative variance of the dose deposited in the site by ions
$V_E$	relative variance of the total energy deposited in the site
$V_F$	relative variance of Fano fluctuations
$V_{F,e}$	relative variance of Fano fluctuations due to electrons
$V_{F,ion}$	relative variance of Fano fluctuations due to ions
$V_L$	relative variance of the LET distribution in the site
$V_{L,e}$	relative variance of the electron LET distribution in the site
$V_{L,ion}$	relative variance of the ion LET distribution in the site
$V_N$	relative variance of the number of events in the site
$V_s$	relative variance of the path length distribution in the site
$V_{s,e}$	relative variance of the electron path length distribution in the site
$V_{s,ion}$	relative variance of the ion path length distribution in the site
$V_{str}$	relative variance of the energy-loss straggling distribution in the site
$V_{str,e}$	relative variance of the energy-loss straggling distribution of electrons in the site
$V_{str,ion}$	relative variance of the energy-loss straggling distribution of ions in the site
$V_\delta$	relative variance of the energy deposited in the site by one collision
$V_\epsilon$	relative variance of the energy deposited in the site by one particle
$V_0$	volume of the site
$V_1$	single event relative variance
$V_{1,e}$	single event relative variance of electrons
$V_{1,ion}$	single event relative variance of ions
$var_F(\epsilon)$	variance of Fano fluctuations
$var_{L,s}(\epsilon)$	variance of $\epsilon$ due to $L$ and $s$
$var_{str}(\epsilon)$	variance of $\epsilon$ due to energy-loss straggling
$\bar{w}$	average energy required to produce one electron-hole pair in the site
$\bar{w}_e$	average energy required for electrons to produce one electron-hole pair in the site
$\bar{w}_{ion}$	average energy required for ions to produce one electron-hole pair in the site
$w(x)$	probability density function for a weighted distribution
$x$	general, continuous random variable
$x_A$	continuous random variable of the $A$ -distribution
$x_B$	continuous random variable of the $B$ -distribution
$\bar{x}_w$	weighted average of $x$
$y$	lineal energy
$\bar{y}_D$	dose mean lineal energy
$\bar{y}_{D,e}$	dose mean lineal energy for electrons
$\bar{y}_{D,ion}$	dose mean lineal energy for ions
$\bar{y}_F$	frequency mean lineal energy
$\bar{y}_{F,e}$	frequency mean lineal energy for electrons
$\bar{y}_{F,ion}$	frequency mean lineal energy for ions
$z$	specific energy (in section D1a); otherwise, specific energy per event
$\bar{z}_D$	dose mean specific energy per event

$\overline{z_{D,e}}$	dose mean specific energy per electron event
$\overline{z_{D,ion}}$	dose mean specific energy per ion event
$\overline{z_F}$	frequency mean specific energy per event
$\overline{z_{F,e}}$	frequency mean specific energy per electron event
$\overline{z_{F,ion}}$	frequency mean specific energy per ion event
$\delta$	energy deposited by a particle in the site by one collision
$\delta_e$	energy deposited by an electron in the site by one collision
$\delta_{ion}$	energy deposited by an ion in the site by one collision
$\epsilon$	energy deposited in the site by one particle
$\epsilon_e$	energy deposited in the site by one electron
$\epsilon_{ion}$	energy deposited in the site by one ion
$\eta$	number of electron-hole pairs produced in the site by one particle
$\eta_e$	number of electron-hole pairs produced in the site by one electron
$\eta_{ion}$	number of electron-hole pairs produced in the site by one ion
$\rho_0$	density of the material composing the site

# ENERGY DEPOSITION FLUCTUATIONS INDUCED BY IONS IN MICROVOLUMES AND NANOVOLUMES — AN ANALYTIC APPROACH

## I. THEORY

### I. INTRODUCTION

The spatial distribution of radiation energy deposited on a micrometer to nanometer scale is central to understanding radiation effects in biological systems<sup>1,2</sup> and modern microelectronics.<sup>3</sup> Because of the essential granular nature of all radiation, energy deposition in small volumes is a statistical process so that knowledge of the macroscopically measured dose does not determine the energy imparted to a particular small volume. Monte Carlo simulations have been the traditional method to model energy deposition by ions in sites whose dimensions are less than approximately one micrometer. Although such simulations have proven to be valuable, they involve sophisticated computer codes and time consuming scoring techniques, require large quantities of input information, tend to be inflexible, and are often tedious to interpret in terms of the relative effects of various input parameters. Consequently, certain aspects of radiobiological and microelectronic studies are difficult to address with Monte Carlo calculations. On the other hand, an analytical approach can provide information to supplement Monte Carlo results, and is more suited to analyze the wide ranges of conditions often encountered in radiation studies.

Experiments in radiobiological research, for example, are commonly performed with a variety of ions and energies to cover a broad range of Linear Energy Transfer (LET). There are also uncertainties associated with the dimensions and geometry of the sensitive site. The dimensions may vary anywhere from the size of a cell nucleus (micrometers) to that of a DNA molecule (nanometers), and the geometry is determined accordingly. By contrast, Monte Carlo calculations have been mainly limited to proton irradiations of sites with a spherical geometry. Furthermore, in specific cases such as radiation-induced DNA damage, it is not generally agreed upon whether energy deposition (ionization plus excitation) or simply electron-hole pair production (ionization) is the relevant quantity related to the damage mechanism. Adjustments of this nature in Monte Carlo codes are difficult to make.

The situations which occur in radiation effects research on microelectronics have related concerns. A variety of ions are commonly used in experiments, and the sensitive volumes of targets involve different materials (Si, GaAs, SiO<sub>2</sub>), dimensions (nanometers to 10's of micrometers) and geometries associated with depletion, diffusion and insulating regions of devices. It is clear that there is a need for a general method which can quickly determine the effects that basic input parameters have on the overall outcome of irradiating very small volumes of matter with ions. This work presents such a method for calculating energy deposition fluctuations which is analytical, based on first principles and whose basic equations do not involve fitted parameters.

The basic derivations are presented in Section II. Some background in statistical terminology is reviewed in IIA, and then a new derivation of relations introduced by Kellerer is presented in IIB. This relates the energy deposition fluctuations caused by a single type of event to the first and second moments of three fundamental distributions. In IIC, the relations are generalized to the "Two Component Model", which analytically describes ion induced energy

deposition fluctuations for dimensions as small as one nanometer. In these sections, the methods are presented in terms of standard statistical quantities such as variances, relative variances and moments of distributions. The microdosimetry literature, however, has evolved using somewhat different terminology. In IID, the relation of this terminology to discussion in previous sections is shown. Those readers not interested in this section can simply omit it without any loss of continuity. Section IIE gives, with the aid of flow charts, an overview of the ideas behind the Two Component Model. Finally, section III is a brief summary.

## II. THEORY

### A. Review of the Statistics of Continuous Random Variables

In much of what follows, it will be useful to parameterize the distribution of values which a random variable can assume in terms of its relative variance and in terms of the moments of the distribution. Suppose  $x$  is a continuous random variable described by a probability density function  $f(x)$  that gives the probability of the number of occurrences of  $x$ . Then  $f(x)dx$  represents the probability that the random variable  $x$  is between  $x$  and  $x + dx$ . The first moment of  $x$ , the average, is given by

$$\overline{x} = \int_{-\infty}^{\infty} x \cdot f(x) dx \quad (1)$$

where the overlining of  $x$  indicates it is an average. In general, the  $m^{\text{th}}$  moment of  $x$  is given by

$$\overline{x^m} = \int_{-\infty}^{\infty} x^m \cdot f(x) dx \quad (2)$$

The variance of  $x$ , denoted by  $var(x)$ , is given by

$$var(x) = \sigma_x^2 = \int_{-\infty}^{\infty} (x - \overline{x})^2 \cdot f(x) dx \quad (3)$$

where  $\sigma_x$  is the standard deviation of  $x$ . The variance is also commonly written as the second moment minus the square of the first moment.

$$\text{var}(x) = \overline{x^2} - (\bar{x})^2 \quad (4)$$

The relative variance of the random variable  $x$ ,  $V_x$ , is defined as the variance divided by the square of the average.

$$V_x = \frac{\text{var}(x)}{(\bar{x})^2} \quad (5)$$

Another quantity commonly used to characterize the variability of  $x$  is the coefficient of variation,  $\sigma_x/\bar{x}$ , which is the square root of the relative variance.

Rather than use the average and variance (or relative variance) to describe the distribution of values that  $x$  can assume, it is sometimes more convenient to use the first and second moments of the distribution. A useful relation to know is that between the ratio of the second moment to the first moment of  $x$  and the relative variance of  $x$ . Dividing each side of equation (4) by the square of the average of  $x$ , and making use of equation (5), the moment ratio is easily shown to be given by

$$\frac{\overline{x^2}}{\bar{x}} = \bar{x} \cdot (1 + V_x) \quad (6)$$

There are many other types of probability density functions besides  $f(x)$  that can be employed. One that will be useful, denoted here as  $w(x)$ , describes the probability that the variable  $x$  is a certain value, i.e.,

$$w(x)dx = \frac{x \cdot f(x)dx}{\int x \cdot f(x)dx} \quad (7)$$

In other words,  $w(x)dx$  is the fraction of  $x$  associated with a particular value of  $x$ . This type of distribution is referred to as a weighted distribution. It should be contrasted to the distribution given by  $f(x)$  which describes the number of occurrences of  $x$ . The weighted distribution,  $w(x)$ , is useful for analyzing the concentration of  $x$  rather than its frequency of occurrence.

The average of  $x$  taken over the weighted distribution is

$$\overline{x}_W = \int_{-\infty}^{\infty} x \cdot w(x) dx \quad (8)$$

where the subscript  $W$  is used to indicate it is a weighted average to distinguish it from the arithmetic average given by equation (1). The weighted average can be expressed in terms of  $f(x)$  by substituting equation (7) into equation (8).

$$\overline{x}_W = \frac{\int_{-\infty}^{\infty} x^2 \cdot f(x) dx}{\int_{-\infty}^{\infty} x \cdot f(x) dx} \quad (9)$$

It will be recognized from equation (2) that this weighted average can be expressed as the second moment of  $x$  divided by the first moment of  $x$ .

$$\overline{x}_W = \frac{\overline{x^2}}{\overline{x}} \quad (10)$$

Expressions involving the ratio of the second moment to the first moment of a continuous random variable play a fundamental role in microdosimetry theory because the concentration of the physical quantity which the variable represents can influence the outcome of an irradiation.

## B. Relations between the Random Physical Variables and Energy Deposition Fluctuations

The basic relations describing energy deposition fluctuations for a single type of event such as the traversal of a target site by an ion was introduced originally by Kellerer.<sup>1</sup> However, the origin of the equations is only discussed briefly in this somewhat obscure reference. One problem confronting a reader not familiar with the theory is its apparent isolation from other fields of research. The reason for presenting the following derivation is to make clear the principles behind the equations so that the model which is developed from these relations can be applied to other physical systems. To this end, a more straight-forward derivation of the basic equations than that outlined in reference 1 is presented.

In section B1, a qualitative description of the random variables important in the energy

deposition process is presented. In B2, the results introduced by Kellerer are obtained from concepts which are well known in stochastic theory. These equations have the random variables expressed in terms of the moments of their distributions. In section B3, the approach is converted to an equivalent one in which the random variables are described by the relative variance of the appropriate distribution.

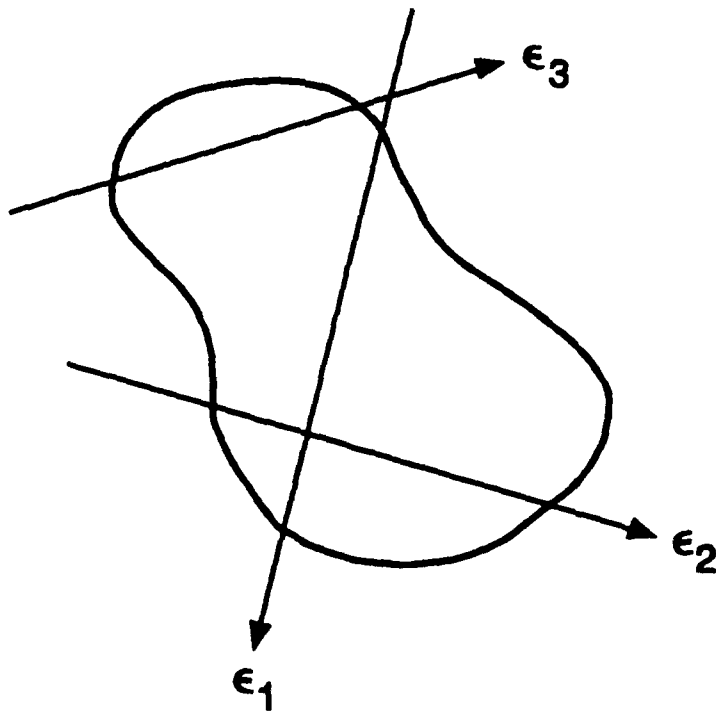
## 1. Random Physical Variables in the Energy Deposition Process

Figure 1a gives an overall view of the energy deposition process. Ions are considered to traverse a small volume of material in straight paths without losing a significant portion of their energy in the volume. The paths are indicated by arrows and the particular situation shown is for a site with an arbitrary geometry crossed by three particles. More generally, the number of particles which traverse the site,  $N$ , is subject to statistical fluctuations.  $N$  is also referred to as the number of events which occur in the site. The particles are assumed to arrive at the site independently and the variability of  $N$  is therefore described by Poisson statistics. More significantly, the energy imparted to the volume by a single particle,  $\epsilon$ , also displays variability and will be discussed below. The overall process is therefore compound Poisson, i.e., a process of  $N$  independent random events of varying magnitude  $\epsilon$ .

Next the random physical variables associated with a single particle traversal of the site are considered. As figure 1b indicates, the particles can have a distribution of LETs as well as a distribution of path lengths through the site. The former is determined by the type and energy of the incident particle while the latter depends on the geometry of the site and the directions from which the particles are incident. The energy deposited by a particle traversing the site depends on the product of the random variables  $L$  and  $s$ .  $L$  is the LET of the particle in the material under consideration and  $s$  is the particle's path length through the site.

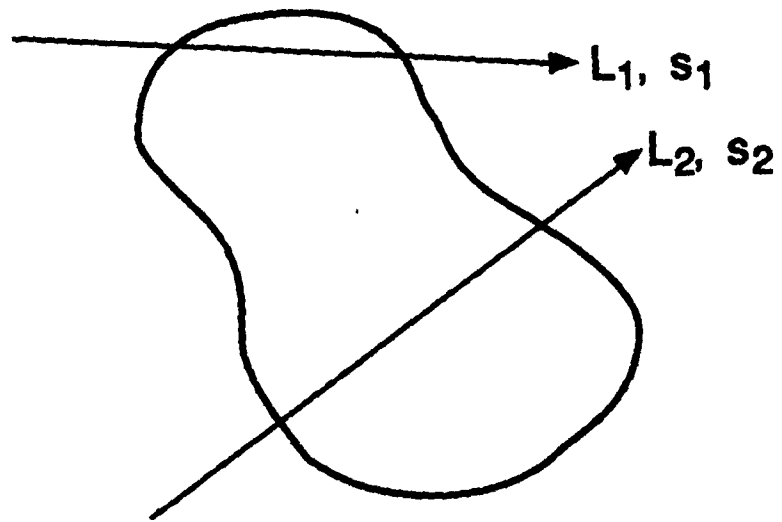
The next process to consider results from fluctuations in the energy deposition for a single particle traversing the site with a fixed LET and a fixed path length. This process is referred to as energy-loss straggling. As the particle crosses the site, it undergoes a random number of collisions with the electrons in the site. The number of collisions or energy transfer points depicted in figure 1c is four and in general is denoted by  $n$ . The collisions occur independently, so  $n$  is described by Poisson statistics. Each collision has a magnitude described by the random variable  $\delta$ , which accounts for both ionizations and inelastic excitations. The energy-loss straggling is also a compound Poisson process because it consists of  $n$  independent events of varying magnitude  $\delta$ . The compound Poisson process therefore plays a role at two levels of the energy deposition process, as has been pointed out previously by Kellerer.<sup>2</sup>

The above discussion considers the random factors contributing to the energy deposited in a small volume of matter which leads in general to both ionizations and inelastic excitations. This may be the quantity of interest, for example, in considering radiation-induced damage in DNA or other polymers. However, a distinction must be made from the situation where the



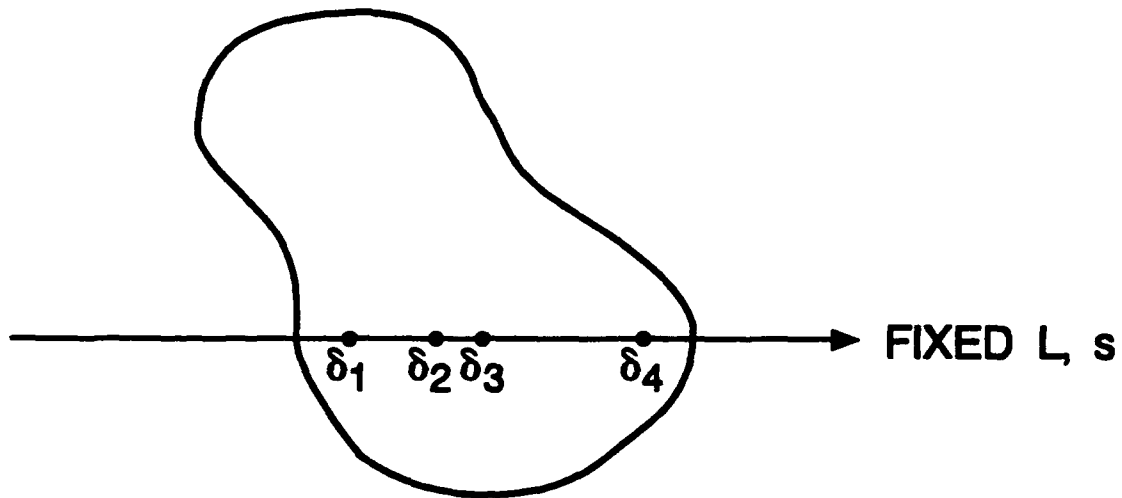
**IN GENERAL:  
N EVENTS – POISSON  
RANDOM MAGNITUDE  $\epsilon$**

Figure 1a. Energy deposition in a small site.



IN GENERAL:  
L RANDOM  
s RANDOM

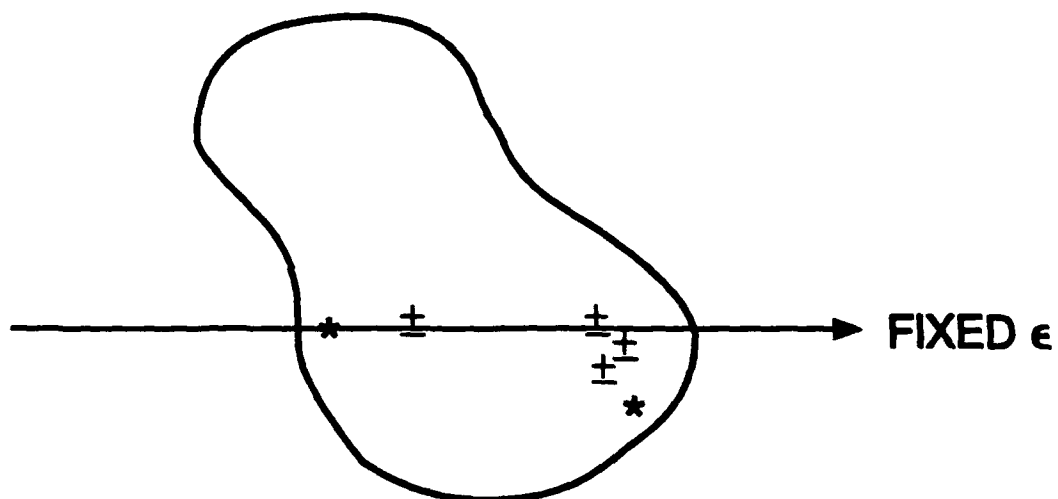
Figure 1b. LET and path length random variables.



- ENERGY TRANSFER POINT

IN GENERAL:  
n COLLISIONS – POISSON  
RANDOM MAGNITUDE  $\delta$

Figure 1c. Energy-loss straggling.



**± ELECTRON - HOLE PAIR**  
**\* INELASTIC EXCITATION**

**IN GENERAL:**  
**η RANDOM**

Figure 1d. Fano fluctuations.

relevant process involves only ionization. This latter situation does not depend on inelastic excitations and is relevant to many types of measurements. Examples include proportional counter spectra used in the microdosimetry field and current-voltage measurements of MOS transistors at low temperatures, which yield information about the distribution of radiation-generated holes in the oxide layer.

Figure 1d shows the random factors involved in converting energy deposited in the volume to ionizations. Consider an ion crossing the site and depositing energy  $\epsilon$ . Each interaction in the site may result in electron-hole pair production (indicated by the paired "+" and "-" signs), inelastic excitations (denoted by asterisks,\*), or both. The statistical partitioning of the energy results in a random number of electron-hole pairs being produced in the site,  $\eta$ . This variability is referred to as Fano fluctuations.<sup>4</sup> The electron-hole pairs are not produced independently, so the process is not Poisson. Fano fluctuations will be considered in more detail in section B2b.

To summarize this section, the discussion involving figure 1a gives an overview of the entire process. Figures 1b and 1c indicate the variability of the energy deposited by a single particle. Finally, figure 1d indicates the additional variability that must be considered to convert energy deposited by a single particle to ionization.

## 2. Energy Deposition Fluctuations with Random Variables Described by Moments

The overall goal of section B2 is to derive the relations introduced by Kellerer which describe the energy deposition fluctuations in a site traversed by an incident particle. For the situation when the incident particle is an ion, the events are commonly referred to in the microdosimetry literature as ion events, direct events or "crossers". The equations depend on the random variables discussed in section B1. The first basic equation, to be derived in B2a, describes the dependence of the fluctuations on the average (or macroscopically measured) dose received by the medium. The second basic equation, obtained in B2b, describes the fluctuations in the energy deposited by a single particle traversing the site.

### a. Dependence of Dose Fluctuations on Average Dose

Assume the target site is struck by a random number of incident ions,  $N$ . The average (or expectation value) of  $N$  is

$$\bar{N} = \sum_{N=0}^{\infty} N \cdot f(N) \quad (11)$$

where  $f(N)$  is the probability that  $N$  ions cross the site. Note that  $f(N)$  is analogous to the

probability density function in equation (1) except that here  $N$  is a discrete random variable.

The total energy deposited in the site,  $E$ , is a random variable given by

$$E = \epsilon_1 + \epsilon_2 + \dots + \epsilon_N \quad (12)$$

where  $\epsilon_i$  denotes the energy deposited by the  $i^{\text{th}}$  of  $N$  total ions. It is assumed that each ion arrives independently. The  $\epsilon_i$  are therefore mutually independent, identically distributed random variables. From equation (4), the variance of the energy deposited by a single particle traversing the site is

$$\text{var}(\epsilon) = \overline{\epsilon^2} - (\overline{\epsilon})^2 \quad (13)$$

The initial objective in this section is to determine the average energy deposited in the site and its variance in terms of the random variables  $\epsilon_i$  and  $N$ .

First, an expression for the average energy deposited will be obtained. Since this quantity depends on both  $\epsilon_i$  and  $N$ , it will be determined by first fixing  $N$  at an arbitrary value of  $N'$ . The average energy is said to be conditional on  $N$ . Its conditional expectation is written

$$\overline{E}|_{N=N'} = \sum_{i=1}^{N'} \overline{\epsilon_i} \quad (14)$$

The left-hand side of equation (14) denotes the average value of  $E$  with  $N$  held at  $N'$ . Its value is obtained by summing the average energy deposited in the site by particles 1 through  $N'$ . The random variables  $\epsilon_i$  are independent and identically distributed so,

$$\overline{\epsilon_{i+1}} = \overline{\epsilon_i} = \overline{\epsilon} \quad (15)$$

That is all the  $\overline{\epsilon_i}$  are equal. Equation (14) can then be written

$$\bar{E}|_{N=N'} = N' \cdot \bar{\epsilon} \quad (16)$$

Now the expression for the average total energy,  $\bar{E}$ , can be obtained by weighting its conditional expectation, and summing over all possible values of  $N'$ . This summation gives

$$\bar{E} = \sum_{N'=0}^{\infty} N' \cdot \bar{\epsilon} \cdot f(N') \quad (17)$$

Since  $\bar{\epsilon}$  is independent of  $N'$ , it can be taken outside the summation. Furthermore,  $N'$  is simply a dummy variable for  $N$ . Making use of these facts and equation (11) gives the result

$$\bar{E} = \bar{\epsilon} \cdot \bar{N} \quad (18)$$

This indicates the expected result that the average energy deposited in the site is the product of the average energy deposited per event and the average number of events.

Next the variance of the energy deposited in the volume will be determined. With the average value of  $E$  now known, its variance can be obtained using

$$\overline{E^2} = \text{var}(E) + (\bar{E})^2 \quad (19)$$

once the second moment of  $E$  is determined. Using an analogous procedure to that above,  $N$  is set equal to a fixed  $N'$  to obtain the conditional expectation of the average of the square of  $E$ .

$$\overline{E^2}|_{N=N'} = \text{var}(E)|_{N=N'} + (\bar{E})^2|_{N=N'} \quad (20)$$

The second term on the right hand side of equation (20) is known from (16). The first term can be evaluated making use of the properties that the  $\epsilon_i$  are independent and identically distributed random variables. First of all, because the  $\epsilon_i$  are independent, the variance contributed by  $N'$  particles is the sum of the individual variances, i.e.,

$$\text{var}(E)|_{N=N'} = \sum_{i=1}^{N'} \text{var}(\epsilon_i) \quad (21)$$

Furthermore, because the  $\epsilon_i$  are identically distributed, (21) simplifies to

$$\text{var}(E)|_{N=N'} = N' \cdot \text{var}(\epsilon) \quad (22)$$

Substituting the results of equations (16) and (22) into the right-hand side of (20),

$$\overline{E^2}|_{N=N'} = N' \cdot \text{var}(\epsilon) + (N')^2 \cdot (\bar{\epsilon})^2 \quad (23)$$

As before, the conditional expectation must be weighted by  $f(N')$  and summed over all possible values of  $N'$  to obtain the average. The average of the square of the energy deposited in the site is therefore given by

$$\overline{E^2} = \sum_{N'=0}^{\infty} [N' \cdot \text{var}(\epsilon) + (N')^2 \cdot (\bar{\epsilon})^2] \cdot f(N') \quad (24)$$

Equation (24) is easily simplified to give

$$\overline{E^2} = \text{var}(\epsilon) \cdot \bar{N} + (\bar{\epsilon})^2 \cdot \overline{N^2} \quad (25)$$

Substituting the expressions for the first and second moments of  $E$  given by (18) and (25), respectively, into (19) gives the variance of  $E$ .

$$\text{var}(E) = \text{var}(\epsilon) \cdot \bar{N} + (\bar{\epsilon})^2 \cdot [\overline{N^2} - (\bar{N})^2] \quad (26)$$

From the definition of variance given by equation (4), equation (26) can also be written

$$\text{var}(E) = \text{var}(\epsilon) \cdot \bar{N} + (\bar{\epsilon})^2 \cdot \text{var}(N) \quad (27)$$

This result is equivalent to Burgess' variance theorem or simply the variance theorem<sup>5</sup>, which is well known in stochastic theory as the basic expression for determining the variance of a sum of a random number of random variables.<sup>a</sup>

As discussed in section B1, the number  $N$  of random variables  $\epsilon$  which make up the sum in equation (12) is controlled by Poisson statistics. A variable controlled by Poisson statistics has the property that its variance is equal to its average value, so

$$\text{var}(N) = \bar{N} \quad (28)$$

Substituting (28) into (27) results in

$$\text{var}(E) = \bar{N} \cdot [\text{var}(\epsilon) + (\bar{\epsilon})^2] \quad (29)$$

Using equation (13), this can be further simplified to give

$$\text{var}(E) = \bar{N} \cdot \bar{\epsilon}^2 \quad (30)$$

The initial objective is now complete. Equations (18) and (30) give the average and the variance of the energy deposited in the site, respectively, in terms of the random variables  $N$  and  $\epsilon$ . It should be noted that the particularly simple form of (30) is a direct result of the fact that energy deposition in a small site is a compound Poisson process. The total variance of such a process depends only on the average number of events and the second moment of the distribution of single events.

Next, these results will be used to determine the variability of the dose deposited in the small volume as a function of the average dose. Dividing equation (30) by the square of equation (18) gives the relative variance of  $E$ ,  $V_E$ .

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<sup>a</sup> Another equivalent form of Burgess' variance theorem can be obtained by converting the three variances in equation (27) to relative variances. The result is  $V_E = V_N + V_\epsilon/\bar{N}$ . Breitenberger (reference 11) gives this form of the result for what he refers to as two processes in "cascade".

$$V_E = \frac{\text{var}(E)}{(\bar{E})^2} = \frac{\overline{\epsilon^2}}{(\bar{\epsilon})^2 \cdot \bar{N}} \quad (31)$$

Using (18) to eliminate the dependence on  $\bar{N}$  results in

$$V_E = \frac{\overline{\epsilon^2}}{\bar{E} \cdot \bar{\epsilon}} \quad (32)$$

In evaluating (32),  $\epsilon$  and  $E$  must have the same energy units. In microdosimetry calculations,  $\epsilon$  typically is in keV. However, the energy deposited in the site,  $E$ , is commonly referred to in terms of radiation absorbed dose (rad) units. (1 rad = .01 Gray = 100 erg/g) The appropriate conversion is:

$$D = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot E \quad (33)$$

where  $E$  is in keV and  $D$  is the corresponding dose in rads.  $V_0$  is the volume of the site in  $\text{cm}^3$  and  $\rho_0$  is the density in  $\text{g}/\text{cm}^3$ . Since  $D$  is proportional to  $E$ , it follows that the relative variance of  $D$ ,  $V_D$ , equals the relative variance of  $E$ ,  $V_E$ . Using this equivalence in equation (32), and making use of equation (33) to express  $E$  in terms of rad units, equation (32) becomes

$$V_D = \frac{1}{\bar{D}} \cdot \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \frac{\overline{\epsilon^2}}{\bar{\epsilon}} \quad (34)$$

where  $\epsilon$  is in keV and  $D$  in rads.  $V_D$  is the relative variance of the dose deposited in the site. Furthermore, recall that  $\epsilon$  is the energy deposited in the site by a single ion, which is independent of dose. The right hand side of (34) is therefore the product of a dose independent factor and the reciprocal of the average dose. Denoting the dose independent quantity by  $\bar{z}_D$ , this can be written

$$V_D = \frac{\bar{z}_D}{\bar{D}} \quad (35)$$

where  $\bar{z}_D$  is given by (36) below. Equation (35) is the final result of this section. It describes the relative variance of the dose deposited in a small volume as a function of the average or macroscopically measured dose. As noted in IIA, a relative variance can be converted to a variance by multiplying by the square of the average or to a coefficient of variation by taking its square root. The quantity  $\bar{z}_D$  will be discussed in detail in the following section.

The main results of this section can be summarized as follows. Equations (18) and (27) give the average and variance of  $E$ , respectively, in terms of the random variables  $\epsilon$  and  $N$ . Equation (27) is also equivalent to Burgess' variance theorem or the variance theorem. If it is assumed that the variable  $N$  is controlled by a Poisson process, then the more general equation (27) reduces to equation (30), which describes a compound Poisson process. Equation (30) can be algebraically manipulated to obtain equation (35), which expresses the relative variance of the dose deposited in a small site in terms of the average dose.

### b. Fluctuations in Dose due to Single Ion Events

Comparing equations (34) and (35) it is seen that the dose independent quantity denoted by  $\bar{z}_D$  is given by

$$\bar{z}_D = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \frac{\bar{\epsilon}^2}{\bar{\epsilon}} \quad (36)$$

Equation (36) can also be written as

$$\bar{z}_D = \frac{\bar{d}^2}{\bar{d}} \quad (37)$$

where  $d$  is the dose deposited in the site by a single ion. In the microdosimetry literature,  $\bar{z}_D$  is called the dose mean specific energy per event.<sup>6</sup> It is the ratio of the second moment to the first moment of the dose deposited in the site due to single events. Note from equation (10) that it can be regarded as a weighted average of the dose deposited by single events. As is customary, the subscript  $D$  indicates a dose weighted average. The dose mean specific energy per event is further described and interpreted in section D1 in terms of probability density functions. It should also be noted from equation (6) that  $\bar{z}_D$  contains the information describing the variability of the interaction of a single particle with the site.

The purpose of this section is to derive an expression for the dose mean specific energy per event in terms of the random physical variables described in B1. The final expression will

depend on variables associated with the LET, path length and collision magnitude of ions in the site, which are denoted by  $L$ ,  $s$  and  $\delta$ , respectively. The distributions of these random variables are assumed to be in the form of the ratio of the second to the first moment of the respective distribution. Additionally, it will be shown how to convert the description of the fluctuations in the total energy deposited in the site to one which describes the fluctuations of the ionization process.

First of all, consider the variability associated with the LET,  $L$ , and path length,  $s$ , variables for a single ion event as shown in figure 1b.  $L$  and  $s$  are independent, so the average of their product is equal to the product of their averages. Furthermore, the product of the two variables is the energy deposited in the site by one ion,  $\epsilon$ .

$$\bar{\epsilon} = \overline{L \cdot s} = \bar{L} \cdot \bar{s} \quad (38)$$

For similar reasons,

$$\overline{\epsilon^2} = \overline{L^2 \cdot s^2} = \overline{L^2} \cdot \overline{s^2} \quad (39)$$

Making use of equation (13), the variance of  $\epsilon$  due to  $L$  and  $s$  is

$$\text{var}_{L,s}(\epsilon) = \overline{L^2 \cdot s^2} - (\bar{L})^2 \cdot (\bar{s})^2 \quad (40)$$

Equation (40) gives the variance of the energy deposited due to the LET distribution of the incident ion and its possible path lengths through the volume. However, the energy deposited by a single ion would fluctuate even if  $L$  and  $s$  were constant. The next step, therefore, is to determine the variance contributed by these fluctuations, which are due to energy-loss straggling as discussed in section B1.

The energy lost in single collisions by the incident ion is described by the random variable  $\delta$  and the number of such collisions in the site by the random variable  $n$ . The process is shown in figure 1c. The total energy deposited by the traversal of the ion is therefore given by the sum

$$\epsilon = \delta_1 + \delta_2 + \dots + \delta_n \quad (41)$$

where  $\delta_i$  denotes the energy lost in the  $i^{\text{th}}$  of  $n$  total collisions. The collisions are assumed to

occur independently so that the  $\delta_i$  are mutually independent, identically distributed random variables. This situation is analogous to that expressed by equation (12). The calculation of the average of  $\epsilon$  and the variance of  $\epsilon$  due to energy-loss straggling,  $var_{str}(\epsilon)$ , in terms of the random variables  $\delta$  and  $n$  is formally the same as the calculations in section B2a and will not be repeated here. The results are

$$\bar{\epsilon} = \bar{\delta} \cdot \bar{n} \quad (42)$$

and

$$var_{str}(\epsilon) = var(\delta) \cdot \bar{n} + (\bar{\delta})^2 \cdot var(n) \quad (43)$$

Equations (42) and (43) are analogous to equations (18) and (27), respectively. The subscript "str" in (43) indicates that the variance results from the straggling process. Continuing the analogy, note that  $n$  is governed by Poisson statistics so (43) can be simplified to a result which is mathematically similar to equation (30).

$$var_{str}(\epsilon) = \bar{n} \cdot \bar{\delta}^2 \quad (44)$$

The notable feature of the two processes described by equations (30) and (44) is that they are both compound Poisson. This results in a similar mathematical description for the total energy deposited in the site and the energy-loss straggling of a single particle.

The variance expressed by (44) due to energy-loss straggling occurs regardless of the LET and path length of the incident ion so the processes are independent. Although this is not a sufficient condition to simply sum the (weighted) variances of the processes, a simple summation can be justified for this situation. Further discussion of this point is provided at the beginning of section C1. The total variance of these two processes is therefore

$$var(\epsilon) = \bar{L}^2 \cdot \bar{s}^2 - (\bar{L})^2 \cdot (\bar{s})^2 + \bar{n} \cdot \bar{\delta}^2 \quad (45)$$

Equation (45) represents the total variance of the energy deposited in the site by a single particle and includes the contributions due to both ionizations and inelastic excitations.

If only the ionization process is of interest, a variance must be added to equation (45)

which accounts for fluctuations in the partitioning of the energy between ionizations and inelastic excitations. Three possible outcomes of the interaction of an incident ion with a bound electron are shown in figure 1d. First of all, the interaction may produce only excitation. Secondly, it may produce only a single ionization. Thirdly, it may produce an ionization in which the resulting electron has kinetic energy. The ejected electron subsequently undergoes interactions which can be ionizations and/or excitations. These three outcomes correspond to the situation in which the energy transferred to the bound electron is less than, equal to and greater than its binding energy, respectively. The result of this energy partition between ionizations and excitations is that even for a fixed amount of energy deposited in the site by a single ion, the number of electron-hole pairs produced fluctuate around an average value. These fluctuations are referred to as Fano fluctuations.

The energy deposited in the site by a single ion can be written in terms of the number of electron-hole pairs produced,  $\eta$ .

$$\epsilon = \bar{w} \cdot \eta \quad (46)$$

where  $\bar{w}$  is the average energy required to produce one electron-hole pair. In this expression,  $\epsilon$  and  $\eta$  are treated as random variables and  $\bar{w}$  as a constant. The average of  $\epsilon$  is then given by

$$\bar{\epsilon} = \bar{w} \cdot \bar{\eta} \quad (47)$$

The corresponding variance of  $\epsilon$  due to Fano fluctuations,  $var_F(\epsilon)$ , is then given by

$$var_F(\epsilon) = (\bar{w})^2 \cdot var(\eta) \quad (48)$$

The Fano factor,  $F$ , is often introduced as an empirical constant by which the Poisson variance of  $\eta$  must be multiplied to give the observed variance of  $\eta$ .<sup>7</sup>

$$var(\eta) = F \cdot \bar{\eta} \quad 0 \leq F \leq 1 \quad (49)$$

For  $F = 1$ , the process is Poisson. For  $F = 0$ , there is no variance, so the same number of electron-hole pairs is always produced. This implies that all the energy is used for ionization. Using equation (49), (48) can be rewritten

$$\text{var}_F(\epsilon) = F \cdot \bar{\eta} \cdot (\bar{w})^2 \quad (50)$$

The Fano fluctuations are assumed to be independent of the fluctuations due to LET, path length and energy-loss straggling and the total variance of the ionization process is taken as the sum of the variances expressed by equations (45) and (50).

$$\text{var}(\epsilon) = \overline{L^2 \cdot s^2} - (\bar{L})^2 \cdot (\bar{s})^2 + \bar{n} \cdot \bar{\delta}^2 + F \cdot \bar{\eta} \cdot (\bar{w})^2 \quad (51)$$

An explanation of why these three variances are simply summed is given at the beginning of section C1. Dividing both sides of (51) by the average energy deposited by a single ion and expressing  $\text{var}(\epsilon)$  in terms of its first and second moments, it is seen that

$$\frac{\overline{\epsilon^2} - (\bar{\epsilon})^2}{\bar{\epsilon}} = \frac{\overline{L^2 \cdot s^2}}{\bar{\epsilon}} - \frac{(\bar{L})^2 \cdot (\bar{s})^2}{\bar{\epsilon}} + \frac{\bar{n} \cdot \bar{\delta}^2}{\bar{\epsilon}} + \frac{F \cdot \bar{\eta} \cdot (\bar{w})^2}{\bar{\epsilon}} \quad (52)$$

Note from (38) that the second terms on each side of the above equation are identical. Therefore,

$$\frac{\overline{\epsilon^2}}{\bar{\epsilon}} = \frac{\overline{L^2 \cdot s^2}}{\bar{\epsilon}} + \frac{\bar{n} \cdot \bar{\delta}^2}{\bar{\epsilon}} + \frac{F \cdot \bar{\eta} \cdot (\bar{w})^2}{\bar{\epsilon}} \quad (53)$$

Substituting the expressions given by (38), (42) and (47) for the average of  $\epsilon$  into the first, second and third terms, respectively, of the right hand side of (53) results in

$$\frac{\overline{\epsilon^2}}{\bar{\epsilon}} = \frac{\overline{L^2}}{\bar{L}} \cdot \frac{\overline{s^2}}{\bar{s}} + \frac{\bar{\delta}^2}{\bar{\delta}} + F \cdot \bar{w} \quad (54)$$

Equation (54) expresses the moment ratio of the energy deposited in the site by single ions in terms of the known moment ratios of the LET, path length and collision magnitude distributions, and known parameters describing the Fano fluctuations. As discussed previously in connection with equation (10), the various moment ratios in equation (54) can be interpreted as weighted averages of the appropriate distribution. Combining this result with equation (36) gives the final expression for the dose mean specific energy per event.

$$\overline{z_D} = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \left( \frac{\overline{L^2}}{\overline{L}} \cdot \frac{\overline{s^2}}{\overline{s}} + \frac{\overline{\delta^2}}{\overline{\delta}} + F \cdot \overline{w} \right) \quad (55)$$

Equations (35) and (55) give the relative variance of the dose deposited in the site in terms of known or calculable quantities. Equation (55) characterizes the variability of a single ion event in the site while the dependence of the relative variance on the average dose is contained entirely in (35). These two equations describe the fluctuations in the ionization process (electron-hole pair production) which occur in the small volume. To describe the relative variance due to the complete energy deposition process, which would include both ionizations and inelastic excitations, the same two equations are used except that the term  $F \cdot \overline{w}$  is set equal to zero in (55). The results derived above are equivalent to those presented by Kellerer.<sup>1,2</sup>

Finally, a note about units in equation (55). The ratio of the second moment to the first moment of the incident particle's LET is in units of keV/ $\mu\text{m}$ , the ratio of the path length moments through the site is in  $\mu\text{m}$ , the ratio of the moments of the distribution of collision magnitudes is in keV,  $F$  is dimensionless,  $w$  is in keV,  $V_0$  is in  $\text{cm}^3$  and  $\rho_0$  is in  $\text{g}/\text{cm}^3$ . The factor of  $1.6 \times 10^{-11}$  simply converts the absorbed dose from keV/g to rads. The dose mean specific energy per event is in rad units.

### 3. Energy Deposition Fluctuations with Random Variables Described by Relative Variances

For some applications it is more convenient to describe the known distributions of the random variables in terms of relative variances rather than in terms of moment ratios. One of the advantages of using relative variances is that they are dimensionless. In section 3a, relations between the moment ratios and relative variances of the pertinent random variables are obtained. Then, using these relations in section 3b, equations (35) and (55) are converted into a form in which the variability of the dose deposited in the site is expressed in terms of relative variances.

#### a. Relations between Moment Ratios and Relative Variances of the Random Variables

In this section, relations between the ratio of the second moment to the first moment and the relative variance are obtained for the LET, path length and energy-loss straggling distributions. Additionally, the term corresponding to the Fano fluctuations in equation (55) is also expressed in terms of its relative variance.

Equation (6) gives the general relation between the relative variance and the moment ratio for a continuous random variable. Applying it to the variables  $L$  and  $s$  results in

$$\frac{\overline{L^2}}{\overline{L}} = \overline{L} (V_L + 1) \quad (56)$$

$$\frac{\overline{s^2}}{\overline{s}} = \overline{s} (V_s + 1) \quad (57)$$

Note that when the variance of  $L$  or  $s$  is zero, the corresponding moment ratio is simply the average value. These limiting cases correspond to the situation of a monoenergetic source of ions, and to the situation where all ion paths through the site have the same length.

As discussed in B1, the energy-loss straggling process itself is a compound Poisson process because the ion undergoes  $n$  independent collisions of varying magnitude  $\delta$  at each collision. The variance of the energy-loss straggling process, given by (44), was obtained by using Burgess' variance theorem to combine the random variables  $n$  and  $\delta$ . The relative variance,  $V_{str}$ , is obtained by dividing the variance by the square of the average. Since the average is given by (42), the relative variance due to energy-loss straggling is

$$V_{str} = \frac{\overline{\delta^2}}{\overline{n} (\overline{\delta})^2} \quad (58)$$

The explicit dependence on the average number of collisions can be eliminated using (42). The relation between the moment ratio of the distribution of collision magnitudes and the relative variance of the straggling process is therefore

$$\frac{\overline{\delta^2}}{\overline{\delta}} = \overline{\epsilon} \cdot V_{str} \quad (59)$$

Although there is no explicit dependence on  $n$  in equation (59), it is understood that  $V_{str}$  is the relative variance for the entire energy-loss straggling process, which includes contributions due to fluctuations in both the number and magnitude of collisions as the ion crosses the site. Although equation (59) is a more useful relation, it is interesting to write  $V_{str}$  in terms of the relative variance of the collision magnitudes,  $V_\delta$ . Applying equation (6) to the variable  $\delta$  and substituting the result into (58), the following equation is obtained.

$$V_{sr} = \frac{1}{n}(1 + V_d) \quad (60)$$

Since  $n$  is governed by Poisson statistics, the first term in (60) is the relative variance of the number of collisions. The second term therefore describes the variability due to the collision magnitudes.

Finally, the term involving the Fano fluctuations in equation (55) will now be related to the relative variance of the Fano fluctuations,  $V_F$ . Equation (50) gives the variance of the fluctuations while (47) gives the average. Again, the relative variance is obtained by dividing the variance by the square of the average.

$$V_F = \frac{F}{\bar{\eta}} \quad (61)$$

This would also follow directly from equation (49). Using (47) to eliminate the dependence on the average number of electron-hole pairs,  $\bar{\eta}$ , the following result is obtained.

$$F \cdot \bar{w} = \bar{\epsilon} \cdot V_F \quad (62)$$

### b. Conversion to the Relative Variance Description

The relations necessary to convert the description with the random variables expressed as moment ratios (equations 35 and 55) to one with the random variables expressed as relative variances are given by (56), (57), (59) and (62). Substituting these relations into equation (55) and with some algebraic manipulation it is seen that

$$\bar{z}_D = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot [\bar{L} \cdot \bar{s} \cdot (V_L + 1) \cdot (V_s + 1) + \bar{\epsilon} \cdot V_{sr} + \bar{\epsilon} \cdot V_F] \quad (63)$$

Noting from (38) that the average LET times the average path length is the average energy deposited by a single ion,  $\bar{\epsilon}$ , this can be written as

$$\bar{z}_D = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \bar{e} \cdot (1 + V_L + V_s + V_L \cdot V_s + V_{sr} + V_F) \quad (64)$$

Recall from (33) that the multiplicative factor  $1.6 \times 10^{-11}/V_0 \cdot \rho_0$  converts energy deposition in keV to dose in rads. Equation (64) can then be expressed as

$$\bar{z}_D = \bar{d} \cdot (1 + V_L + V_s + V_L \cdot V_s + V_{sr} + V_F) \quad (65)$$

where  $\bar{d}$  is the average dose deposited in the site by a single event.

The sum of all the relative variance terms inside the parenthesis on the right hand side of (65) is called the single event relative variance,  $V_1$ .

$$V_1 = V_L + V_s + V_L \cdot V_s + V_{sr} + V_F \quad (66)$$

This quantity is the relative variance of the ionization produced by a single particle in the small volume, excluding that associated with Poisson statistics. It is therefore independent of dose. Writing equation (65) in terms of  $V_1$  gives the useful result

$$\bar{z}_D = \bar{d} (1 + V_1) \quad (67)$$

The next step is to express the relative variance of the dose deposited in the site in terms of  $V_1$ . To accomplish this, (67) is substituted into (35) to obtain

$$V_D = \frac{\bar{d}}{D} \cdot (1 + V_1) \quad (68)$$

Since  $d$  is the dose deposited by a single particle and  $D$  is the total dose, this can be rewritten as

$$V_D = \frac{1}{\bar{N}} \cdot (1 + V_1) \quad (69)$$

where  $\bar{N}$  is the average number of incident ions which strike the site. The mathematical similarity of equations (60) and (69) is apparent. Again, this results from the fact that the energy-loss straggling of an ion crossing a site and the deposition of dose in a site are both compound Poisson processes.

Equations (66) and (69) are the final results. They relate the relative variance of the dose deposited in the site to known relative variances and the average number of incident particles which strike the site. The latter quantity can be calculated from the average deposited dose. Equation (66) characterizes the variability of a single particle interaction in the site and (69) relates the total relative variance to the single event relative variance and the number of events. All quantities in these two equations are dimensionless. Again, these results are equivalent to those presented by Kellerer.<sup>1,2</sup>

Equations (66) and (69), with the Fano fluctuations accounted for by  $V_F$ , describe the fluctuations in the ionization process (electron-hole pair production). To describe the fluctuations due to both ionizations and inelastic excitations, the same two equations are used except that  $V_F$  is set equal to zero in (66).

It is interesting to note two other features of this description using relative variances. First, setting  $V_1 = 0$  in (69), which is equivalent to setting the relative variances due to LET, path length, straggling and Fano fluctuations equal to zero, implies that the relative variance of the dose deposited in the site is described entirely by Poisson statistics. Therefore, the first term in (69) is identified with Poisson fluctuations in the number of particles that strike the site.

Secondly, note that the variability due to  $L$  and  $s$ , which occurs as a result of the product of the two independent random variables, results in three terms involving their relative variances in equation (66). This is the general result for the product of two independent random variables.<sup>1,8</sup> It is usually assumed in texts on statistics that the relative variances are small and an expression is derived from a series expansion which neglects the term involving the product of the two relative variances. The expression presented here is more general and includes the possibility that either or both of  $V_L$  and  $V_s$  can be large.

Finally, note that equation (67) is a convenient expression for converting between the relative variance description given by equations (66) and (69) and the moment ratio description given by equations (35) and (55). It allows the dose mean specific energy per event to be calculated given the single event relative variance,  $V_1$ , or its components  $V_L$ ,  $V_s$ ,  $V_{str}$  and  $V_F$ . Conversely, it allows  $V_1$  to be calculated given the dose mean specific energy per event or the moment ratios of the random variables  $L$ ,  $s$  and  $\delta$ , and the product of the Fano factor and the average energy to produce an electron-hole pair.

### C. The Two Component Model

The relations in section B describe energy deposition fluctuations for a *single type* of event such as the traversal of a site by ions. These relations were published at a time when interest in radiobiology was centered on the micrometer dimensions of cell nuclei. For sub-micrometer dimensions, however, it is no longer sufficient to consider only the incident ions which directly strike the site.<sup>9,10</sup> The range of secondary electrons in the medium can be significant compared to the site dimensions, and energy transfer by electrons into and out of the small volume must be accounted for. In some cases this contribution becomes equally important to that of the direct ion interactions in the site. An electron event (also commonly referred to as an indirect event or a "toucher") is considered to occur when a secondary electron strikes the target site after being created by an incident ion outside of the site. By consideration of both electron and ion events, an approach will be developed to describe energy deposition fluctuations induced by ions in target sites having dimensions as small as one nanometer.

Section 1 gives a review of the appropriate probability theory which will be applied to combine the dose distribution of ions that directly interact with the site and the dose distribution of secondary electrons that interact with the site after being produced by ions in the surrounding medium. The combination of the two distributions is a key part of the derivation which has not been previously addressed in the context of microdosimetry. In section 2, the Two Component Model is obtained for the situation where the random variables of the energy deposition process are described by moments of their respective distributions. Section 3 describes the Two Component Model where the random variables are described by relative variances.

#### 1. Combined or Mixed Probability Distributions

The Two Component Model is based, from a statistical viewpoint, on combining parameters such as the mean and variance of two independent probability distributions to obtain the corresponding parameters of the combined or mixed distribution. It will be necessary to distinguish between the situation where the following analysis of combined probability distributions is applicable and when it is possible to simply sum the weighted variances of the component distributions. Breitenberger<sup>11</sup> makes a clear distinction between the two cases. The analysis of this section applies to what he calls "alternative events". For alternative events, one and only one of two or more possible alternatives will occur in a given trial. As an example in the context of this work, consider the dose deposited in a target site resulting from ion irradiation of the material. An ion may directly strike the site, and this process has an associated dose distribution per event. Alternatively, the ion may miss the site but create a secondary electron which deposits dose in the site. The two independent dose distributions due to ions and electrons result from alternative events, and the variance of the combined distribution is not simply the *sum of the weighted variances of the component distributions*.

On the other hand, it is possible to simply sum the weighted variances for the situation

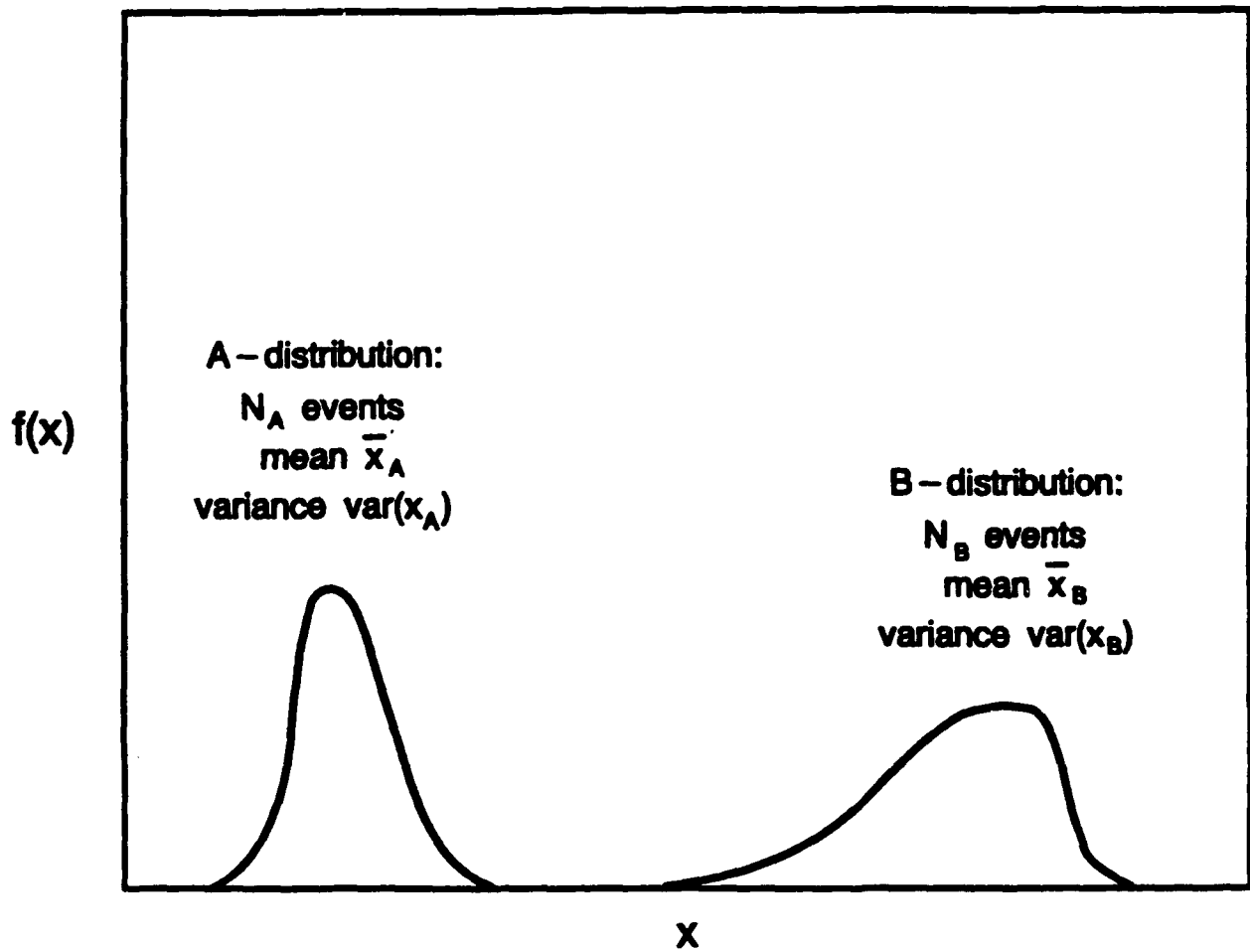


Figure 2. A combined or mixed distribution of "alternative events".

that Breitenberger calls "simultaneous events". Simultaneous events are independent events associated with the same ion that happen at the same time. For example, consider the fluctuations in electron - hole pair production resulting from a single ion event as discussed in section B2b. The three variances which contribute to the fluctuations are due to the LET times the path length of the ion [equation (40)], energy-loss straggling [equation (44)] and Fano fluctuations [equation (50)]. These three processes occur simultaneously and independently as the ion crosses the site. Under these conditions, the total variance is given by (51), which is the sum of the three individual variances.

The following analysis is for a combined probability distribution of alternative events. Consider two independent distributions of continuous random variables  $x_A$  and  $x_B$  shown in figure 2. For clarity, they are shown separated, but they may be overlapping. They will be referred to as the *A*-distribution and the *B*-distribution. The *A*-distribution is made up of  $N_A$  events which have a mean value of  $\bar{x}_A$  and a variance of  $var(x_A)$ . Similarly, the *B*-distribution consists of  $N_B$  events having a mean  $\bar{x}_B$  and a variance  $var(x_B)$ . The ordinate shown in the figure shows the probability density function,  $f(x)$ . It represents the number of events which have a value of  $x$ , normalized to the total number of events,  $N_A + N_B$ . In other words, it is the fraction of the total number of events which have a value of  $x$ . This type of probability function is often called a frequency weighted probability density function in the context of microdosimetry theory and will be elaborated on in section D. It is assumed the means, variances and number of events associated with each component distribution are known. The goal is to combine these known parameters of the two component distributions to arrive at the mean and variance of the overall mixed distribution. Equivalently, the goal is to combine the moments of the component distributions to obtain the moments of the mixed distribution.

The problem of combined or mixed distributions has been treated in the context of applied probability theory by Deming.<sup>12</sup> The basic result for combining moments of the two component distributions is

$$\bar{x}^m = P \cdot \bar{x}_A^m + (1 - P) \cdot \bar{x}_B^m \quad (70)$$

where  $\bar{x}_A^m$  and  $\bar{x}_B^m$  are the  $m^{\text{th}}$  moments of the *A*- and *B*-distributions, respectively, and  $\bar{x}^m$  is the  $m^{\text{th}}$  moment of the mixed distribution. The weighting factors  $P$  and  $1 - P$  are the fraction of the total number of events in the *A*- and *B*-distributions, respectively.

$$P = \frac{N_A}{N_A + N_B} \quad (71)$$

$$1 - P = \frac{N_B}{N_A + N_B} \quad (72)$$

Deming refers to  $P$  and  $1 - P$  as the normalized or relative frequencies of the  $A$ - and  $B$ -distributions.

The average,  $\bar{x}$ , and the variance,  $var(x)$ , of the combined distribution can be obtained making use of equation (70). The average results from setting  $m$  equal to 1.

$$\bar{x} = P \cdot \bar{x}_A + (1 - P) \cdot \bar{x}_B \quad (73)$$

where  $\bar{x}_A$  and  $\bar{x}_B$  are the averages of the  $A$ - and  $B$ -distributions, respectively. The variance of the combined distribution can be obtained by starting with equation (4) and inserting expressions for the first and second moments of  $x$  obtained using equation (70). This gives

$$var(x) = P \cdot \bar{x}_A^2 + (1 - P) \cdot \bar{x}_B^2 - [P \cdot \bar{x}_A + (1 - P) \cdot \bar{x}_B]^2 \quad (74)$$

The first two terms on the right-hand side of equation (74) can be expressed in terms of the average and variance of the appropriate distribution by making use of (4).

$$var(x) = P [var(x_A) + (\bar{x}_A)^2] + (1 - P) [var(x_B) + (\bar{x}_B)^2] - [P \cdot \bar{x}_A + (1 - P) \cdot \bar{x}_B]^2 \quad (75)$$

Note that the variance of the mixed distribution is now written in terms of the averages and variances of the component distributions. All that remains is to simplify equation (75). Expanding the last term and performing some algebraic manipulations, it can be shown that

$$var(x) = P \cdot var(x_A) + (1 - P) \cdot var(x_B) + P \cdot (1 - P) \cdot (\bar{x}_B - \bar{x}_A)^2 \quad (76)$$

This result, along with alternative expressions, is given by Deming. In addition, expressions are given for the variance of an arbitrary number of component distributions. In equation (76),  $var(x_A)$  and  $var(x_B)$  are referred to as the "internal" variances and the last term is called the "external" variance. The variance of the combined distribution is the sum of the internal variances, properly weighted, and the external variance, which is proportional to the square of the separation of the component averages.

In summary, for a combined or mixed distribution of alternative events, equations (70), (73) and (76) give the moments, mean and variance of the combined distribution in terms of known quantities of the independent component distributions. The weighting factors  $P$  and  $1 - P$  are given by (71) and (72), respectively. It has been shown that the correct procedure for this situation is to sum the weighted moments of the component distributions, not the weighted variances. Simply summing the weighted variances is a reasonable approximation only if the averages of the component distributions are nearly equal.

## 2. Energy Deposition Fluctuations with Random Variables Described by Moments

The new microdosimetry model explicitly accounts for two components which contribute to the fluctuations in energy deposited in the site. The components are shown schematically in Figure 3. The first contribution is due to incident ions which directly strike the site. This will subsequently be referred to as the ion or direct component and denoted with the subscript "ion". As shown in the figure, some of the energy initially deposited in the site may be carried out of the site by secondary electrons. The second contribution is due to secondary electrons which strike the site after being created by ions outside the site. This will be referred to as the electron or indirect component and indicated by the subscript "e". This nomenclature and notation is similar to that used previously by Kellerer,<sup>13</sup> the present authors<sup>14</sup> and Olko and Booz.<sup>15</sup> Both the ion and the electron components contribute to the fluctuations in energy deposited in the target site. In order to characterize the overall energy distribution, the means and variances of the ion and electron distributions must be properly combined. The mathematical problem of combining the two probability distributions has been discussed in the previous section.

To begin, note that (69) expresses the total relative variance of the dose in terms of the relative variance due to single events and the average number of events in the site. Using the definition of relative variance given by (5), equation (69) can be written

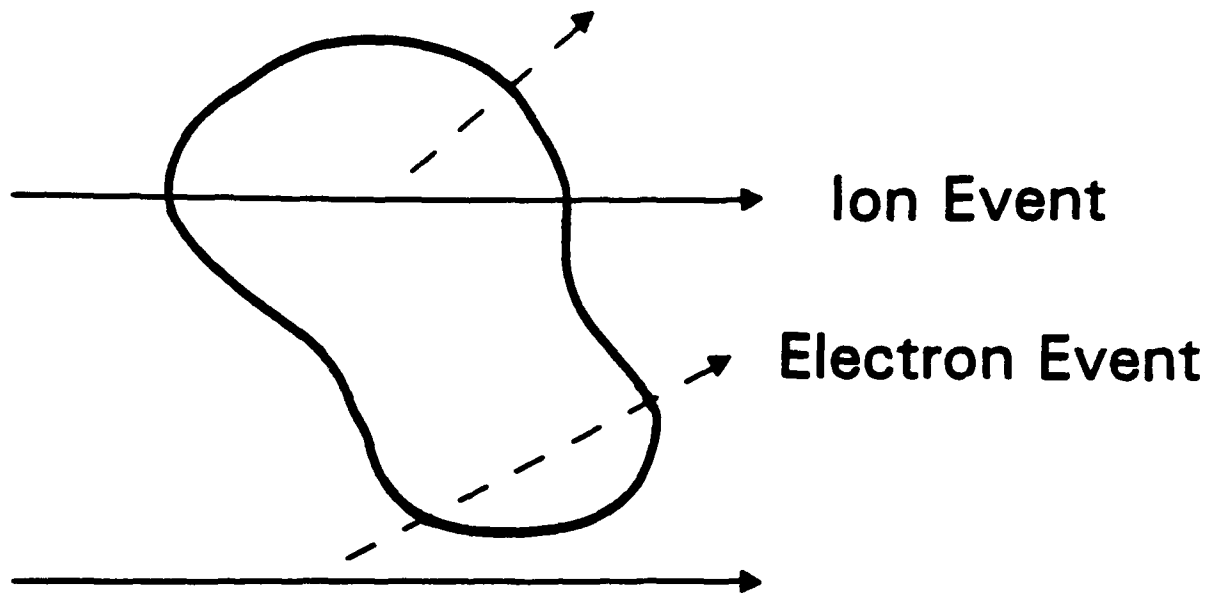
$$\frac{\text{var}(D)}{(\bar{D})^2} = \frac{1}{\bar{N}} \cdot \left[ 1 + \frac{\text{var}(d)}{(\bar{d})^2} \right] \quad (77)$$

where  $\bar{D}$  and  $\text{var}(D)$  are the mean and variance of the total dose deposited in the site, and  $\bar{d}$  and  $\text{var}(d)$  are the mean and variance of the dose deposited by a single particle.

Furthermore, equation (18) can be expressed in terms of dose related quantities.

$$\bar{D} = \bar{d} \cdot \bar{N} \quad (78)$$

Inserting (78) into (77), the variance of the dose can be written as



—————→ Incident Ion  
- - - - -→ Secondary Electron

Figure 3. Factors contributing to energy deposition in the Two Component Model.

$$\text{var}(D) = \bar{N} \cdot [\overline{d^2} + \text{var}(d)] \quad (79)$$

Since the variance of  $d$  is given by

$$\text{var}(d) = \overline{d^2} - (\bar{d})^2 \quad (80)$$

equation (79) simplifies to

$$\text{var}(D) = \bar{N} \cdot \overline{d^2} \quad (81)$$

The variance of the total dose deposited in the site is the product of the average number of events and the second moment of the single event dose distribution.

The problem is to determine an expression for the total variance for the situation where the two multiplicative factors in (81) result from a combined distribution of ion and electron events. The first factor, the average number of total events, is the sum of the average number of ion events and the average number of electron events.

$$\bar{N} = \overline{N}_{ion} + \overline{N}_e \quad (82)$$

The remaining factor, the second moment of the single event dose distribution, is now considered. Any given event, by definition, deposits dose in the site. The dose deposited by this event results from either an ion striking the site or an electron striking the site. There are two independent dose distributions which result from the two types of events. Therefore, as discussed in section C1, the ion and electron events are "alternative" events. Equation (70) can then be applied to combine the  $m^{\text{th}}$  moments of the ion and electron single event dose distributions to obtain the  $m^{\text{th}}$  moment of the overall dose distribution. The result for combining the second moments is

$$\overline{d^2} = P \cdot \overline{d_{ion}^2} + (1 - P) \cdot \overline{d_e^2} \quad (83)$$

where  $d_{ion}$  and  $d_e$  are the dose deposited in the site by single ion and by single electron events, respectively.  $P$  and  $1 - P$  represent the fractions of the total number of events due to ions and electrons, respectively. Equation (81) can now be written as

$$\text{var}(D) = \overline{N} \cdot [P \cdot \overline{d_{ion}^2} + (1 - P) \cdot \overline{d_e^2}] \quad (84)$$

It turns out to be more convenient to express the results in terms of dose fractions rather than the event fractions  $P$  and  $1 - P$ . Next, expressions will be obtained which relate the two types of fractions. The fraction of direct ion hits of the site is, on the average, given by

$$P = \frac{\overline{N_{ion}}}{\overline{N_{ion}} + \overline{N_e}} \quad (85)$$

The corresponding fraction of electron hits is

$$1 - P = \frac{\overline{N_e}}{\overline{N_{ion}} + \overline{N_e}} \quad (86)$$

The dose fractions are given by similar expressions. If  $D_{ion}$  is the dose deposited by ion strikes and  $D_e$  is the dose deposited by electron strikes,

$$f_{ion} = \frac{\overline{D_{ion}}}{\overline{D_{ion}} + \overline{D_e}} \quad (87)$$

$$1 - f_{ion} = \frac{\overline{D}_e}{\overline{D}_{ion} + \overline{D}_e} \quad (88)$$

where  $f_{ion}$  and  $1 - f_{ion}$  are the fractions of dose deposited by the ion and electron components, respectively. Furthermore, if  $d_{ion}$  is the dose deposited per ion event and  $d_e$  is the dose deposited per electron event, then

$$\overline{D}_{ion} = \overline{d}_{ion} \cdot \overline{N}_{ion} \quad (89)$$

$$\overline{D}_e = \overline{d}_e \cdot \overline{N}_e \quad (90)$$

Substituting (89) and (90) into (87) and also into (88) results in

$$f_{ion} = \frac{\overline{d}_{ion} \cdot \overline{N}_{ion}}{\overline{d}_{ion} \cdot \overline{N}_{ion} + \overline{d}_e \cdot \overline{N}_e} \quad (91)$$

$$1 - f_{ion} = \frac{\overline{d}_e \cdot \overline{N}_e}{\overline{d}_{ion} \cdot \overline{N}_{ion} + \overline{d}_e \cdot \overline{N}_e} \quad (92)$$

Dividing the numerator and denominator of these two equations by  $\overline{N}_{ion} + \overline{N}_e$ , they become

$$f_{ion} = \frac{P \cdot \overline{d}_{ion}}{P \cdot \overline{d}_{ion} + (1 - P) \cdot \overline{d}_e} \quad (93)$$

$$1 - f_{ion} = \frac{(1 - P) \cdot \overline{d}_e}{P \cdot \overline{d}_{ion} + (1 - P) \cdot \overline{d}_e} \quad (94)$$

The denominator of the above two expressions is the average value of the dose deposited per event of the combined distribution. This can be seen from equation (73), the general expression for the average of the mixed distribution.

$$\bar{d} = P \cdot \bar{d}_{ion} + (1 - P) \cdot \bar{d}_e \quad (95)$$

Using (95), equations (93) and (94) can be written

$$f_{ion} = \frac{P \cdot \bar{d}_{ion}}{\bar{d}} \quad (96)$$

$$1 - f_{ion} = \frac{(1 - P) \cdot \bar{d}_e}{\bar{d}} \quad (97)$$

These last two expressions are the relations between the event fractions,  $P$  and  $1 - P$ , and the dose fractions,  $f_{ion}$  and  $1 - f_{ion}$ . Solving (96) for  $P$  and (97) for  $1 - P$ , and inserting the results into (84), the variance of  $D$  becomes

$$\text{var}(D) = \bar{N} \cdot \left[ \frac{f_{ion} \cdot \bar{d}}{\bar{d}_{ion}} \cdot \bar{d}_{ion}^2 + \frac{(1 - f_{ion}) \cdot \bar{d}}{\bar{d}_e} \cdot \bar{d}_e^2 \right] \quad (98)$$

Equation (78) can be used to write this in terms of the average dose, which is a measurable quantity.

$$\text{var}(D) = f_{ion} \cdot \bar{D} \cdot \frac{\bar{d}_{ion}^2}{\bar{d}_{ion}} + (1 - f_{ion}) \cdot \bar{D} \cdot \frac{\bar{d}_e^2}{\bar{d}_e} \quad (99)$$

Recall from (37) that the dose mean specific energy per event is the ratio of the second moment to the first moment of the dose deposited by a single particle in the site. It is natural, then, to identify the two moment ratios in the above equation as analogous quantities for ions and

electrons.

$$\overline{z_{D,ion}} = \frac{\overline{d_{ion}^2}}{\overline{d_{ion}}} \quad (100)$$

$$\overline{z_{D,e}} = \frac{\overline{d_e^2}}{\overline{d_e}} \quad (101)$$

In microdosimetry terminology, equation (100) represents the dose mean specific energy per event for direct ion strikes of the site, and (101) is the analogous quantity for electron strikes. These two quantities are further described and interpreted in section D.

The variance given by (99) can now be written

$$\text{var}(D) = f_{ion} \cdot \overline{D} \cdot \overline{z_{D,ion}} + (1 - f_{ion}) \cdot \overline{D} \cdot \overline{z_{D,e}} \quad (102)$$

This can be converted to a relative variance by dividing both sides of (102) by the square of the average deposited dose.

$$V_D = \frac{f_{ion} \cdot \overline{z_{D,ion}} + (1 - f_{ion}) \cdot \overline{z_{D,e}}}{\overline{D}} \quad (103)$$

This result can be compared to equation (35). It is seen that in order to obtain the total relative variance of the dose, the dose mean specific energies of ions and electrons must be weighted by the fraction of dose deposited in the site by each type of event.

When  $f_{ion}$  is close to unity, the ion component dominates. For this situation nearly all the energy initially deposited in the site remains within it. As the energy transfer by secondary electrons into and out of the site becomes significant,  $f_{ion}$  becomes less than one, and the electron component becomes more important. Intuitively, it would be expected that the electron component would be most important for small site dimensions and for high energy incident ions.

The dose mean specific energies per event for ions and electrons are obtained by applying

equation (55) to each type of event.

$$\overline{z_{D,ion}} = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \left( f_{ion} \frac{\overline{L_{ion}^2}}{\overline{L_{ion}}} \cdot \frac{\overline{s_{ion}^2}}{\overline{s_{ion}}} + \frac{\overline{\delta_{ion}^2}}{\overline{\delta_{ion}}} + F_{ion} \cdot \overline{w_{ion}} \right) \quad (104)$$

$$\overline{z_{D,e}} = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \left( \frac{\overline{L_e^2}}{\overline{L_e}} \cdot \frac{\overline{s_e^2}}{\overline{s_e}} + \frac{\overline{\delta_e^2}}{\overline{\delta_e}} + F_e \cdot \overline{w_e} \right) \quad (105)$$

where  $L_{ion}$  and  $L_e$  are the random variables which represent the LET of the incident ion and incident secondary electron, respectively,  $s_{ion}$  and  $s_e$  are the path lengths of the ion and electron in the site,  $\delta_{ion}$  and  $\delta_e$  represent the energy deposited in a single ion collision and a single electron collision in the site,  $F_{ion}$  and  $F_e$  are the Fano factors for the two components,  $\overline{w_{ion}}$  and  $\overline{w_e}$  are the average energies required to produce one electron-hole pair by each component,  $V_0$  is the volume of the site and  $\rho_0$  its density. The presence of the factor  $f_{ion}$  in equation (104) accounts for transport of energy initially within the site to the outside, as indicated in figure 3. An analogous factor is not present in equation (105) because the overwhelming majority of incident secondary electrons do not create tertiary electrons within the site with sufficient energy to escape.<sup>16</sup>

The last term in each of (104) and (105) is associated with the Fano fluctuations of the ion and electron components, respectively. Setting them equal to zero results in a description of the energy deposition (ionizations and excitations) in the site while including them describes the ionization (electron-hole pair production) in the site. The Fano fluctuations are a very small contribution for micrometer-sized sites.<sup>2</sup> However, they can become significant as site dimensions approach nanometers.

Equations (103), (104) and (105) are the basic equations for the Two Component Model when the distributions associated with the random variables for the ion and electron components are given in terms of moment ratios. The latter two equations describe the interaction of single particles (ions and electrons, respectively) with the site. Equation (103) weights the two components properly and accounts for the average dose dependence of the fluctuations.

### 3. Energy Deposition Fluctuations with Random Variables Described by Relative Variances

In the discussion of section B, it was noted that the mathematical manipulation may be easier if the contributions to the fluctuations are described in terms of relative variances rather than moment ratios. In this section, the moment ratio description of the previous section is

converted to a form in which the random variables associated with the Two Component Model are given as relative variances. Note that upon inspection of equation (103), the total relative variance of the dose deposited is the sum of the relative variances due to the ion and electron components. In transforming to the relative variance description, it will be simpler to consider each component relative variance separately. Denoting them by  $V_{D,ion}$  and  $V_{D,e}$ ,

$$V_{D,ion} = \frac{f_{ion} \cdot \overline{z_{D,ion}}}{\overline{D}} \quad (106)$$

$$V_{D,e} = \frac{(1 - f_{ion}) \cdot \overline{z_{D,e}}}{\overline{D}} \quad (107)$$

To convert the Two Component Model to a description based on relative variances, equation (67) is a convenient starting point. Applying it to the ion component,

$$\overline{z_{D,ion}} = \overline{d_{ion}} \cdot (1 + V_{1,ion}) \quad (108)$$

where  $d_{ion}$  is the dose deposited in the site by a single ion, allowing for transport of energy initially within the site to the outside, and  $V_{1,ion}$  is the corresponding relative variance due to these single events. In analogy to (66),  $V_{1,ion}$  is given by

$$V_{1,ion} = V_{L,ion} + V_{s,ion} + V_{L,ion} \cdot V_{s,ion} + V_{str,ion} + V_{F,ion} \quad (109)$$

where  $V_{L,ion}$ ,  $V_{s,ion}$ ,  $V_{str,ion}$  and  $V_{F,ion}$  are the relative variances of LET, path length, straggling and Fano fluctuations for the incident ions. Substituting (108) into (106) gives the following

$$V_{D,ion} = \frac{f_{ion} \cdot \overline{d_{ion}}}{\overline{D}} \cdot (1 + V_{1,ion}) \quad (110)$$

In analogy to equation (69), the factor in front of the parenthesis will be expressed in terms of the average number of ion events. This quantity is equal to the fraction of the average dose

deposited by ions divided by the average dose deposited per ion event.

$$\overline{N_{ion}} = \frac{f_{ion} \cdot \overline{D}}{\overline{d_{ion}}} \quad (111)$$

Combining (110) and (111) results in

$$V_{D,ion} = \frac{f_{ion}^2}{N_{ion}} \cdot (1 + V_{1,ion}) \quad (112)$$

This expression gives the relative variance of the dose deposited in the site by ions in terms of dimensionless quantities.

A similar procedure can be used to obtain the relative variance of the dose deposited in the site by secondary electrons. Applying (67) to the secondary electrons

$$\overline{z_{D,e}} = \overline{d_e} \cdot (1 + V_{1,e}) \quad (113)$$

where  $d_e$  is the dose deposited in the site by a single electron created outside of it.  $V_{1,e}$  is the relative variance due to these single electron events and is given by

$$V_{1,e} = V_{L,e} + V_{s,e} + V_{L,e} \cdot V_{s,e} + V_{str,e} + V_{F,e} \quad (114)$$

$V_{L,e}$ ,  $V_{s,e}$ ,  $V_{str,e}$  and  $V_{F,e}$  are the relative variances of the LET, path length, straggling and Fano fluctuations of the incident electrons. Substituting (113) into (107) results in

$$V_{D,e} = \frac{(1 - f_{ion}) \cdot \overline{d_e}}{\overline{D}} \cdot (1 + V_{1,e}) \quad (115)$$

The average number of electron events is given by

$$\bar{N}_e = \frac{(1 - f_{ion}) \cdot \bar{D}}{\bar{d}_e} \quad (116)$$

Equation (115) can now be rewritten in terms of dimensionless quantities by making use of (116).

$$V_{D,e} = \frac{(1 - f_{ion})^2}{\bar{N}_e} \cdot (1 + V_{1,e}) \quad (117)$$

This gives the relative variance of the dose deposited in the site by the electron component. The two terms of equation (103) associated with the relative variance of the ion and electron components, properly weighted, are now given by (112) and (117), respectively. The total relative variance is therefore given by their sum.

$$V_D = \frac{f_{ion}^2}{\bar{N}_{ion}} \cdot (1 + V_{1,ion}) + \frac{(1 - f_{ion})^2}{\bar{N}_e} \cdot (1 + V_{1,e}) \quad (118)$$

Equations (109), (114) and (118) are the basic relations for evaluating the fluctuations of electron-hole pair production in the site, given that the basic information of the random variables is in the form of relative variances. Equations (109) and (114) account for the variability of the ionizations in the site produced by single incident ions and single incident electrons, respectively. Equation (118) properly weights the two components and incorporates the average dose dependence in terms of the number of ion and electron events. If energy fluctuations are the quantity of interest instead of ionizations,  $V_{F,ion}$  and  $V_{F,e}$  are set equal to zero in (109) and (114), respectively.

Equations (109), (114) and (118) are particularly well suited for evaluating the relative contributions of the various physical factors which contribute to the energy deposition (or electron-hole pair) fluctuations. The total relative variance can be broken into contributions due to ion and electron events. Furthermore, the contributions due to the LET distribution, path length distribution, straggling distribution, Fano fluctuations and Poisson statistics for both ion and electron events can be analyzed.

## D. Microdosimetric Quantities and the Two Component Model

The microdosimetry literature has evolved using somewhat different terminology than that used up to this point. The concepts in this literature can also be applied to other fields of research. However, their unfamiliarity to someone outside the field can make reading the literature difficult. The purpose of section D is to show how the most important of the microdosimetric quantities are described by the Two Component Model. At the same time, the rationale behind them will be presented and they will be related to the more common terminology in previous sections. D1 discusses specific energy related quantities and D2 discusses lineal energy related quantities. The specific energy and lineal energy are the microscopic analogues of dose and LET, respectively.

### 1. Specific Energy Related Quantities

#### a. Definition and Background

The term specific energy was originally introduced to distinguish between the process of dose deposition on a microscopic scale and the traditional concept of dose, which is a macroscopic, average quantity. The specific energy is defined as the energy imparted by ionizing radiation to a small volume divided by the mass of the volume. This definition is similar to that of dose but it is recognized that specific energy is a quantity which refers to localized dose deposition and has a stochastic nature. The word "localized" is emphasized to distinguish between the energy lost by radiation as it interacts with a site and the energy deposited in the site. In microdosimetry theory, specific energy is represented by  $z$ . In previous sections the symbol  $D$  has been used to represent the same quantity with an overlined  $D$  indicating an average value. Specific energy distributions are often described formally using probability density functions. Two kinds of probability density functions have proven to be of interest in microdosimetry. The first weights a quantity's value by the fraction of occurrences of that value. This is called a frequency weighted probability density function. The second weights a quantity's value by the fraction of dose associated with that value. This is called a dose weighted probability density function. The frequency weighted probability density function associated with specific energy is denoted by  $f(z)$  and can be thought of as an event frequency spectrum. The fraction of specific energy occurrences between  $z$  and  $z + dz$  is  $f(z)dz$ . The dose weighted probability density function associated with specific energy is denoted by  $d(z)$  and can be thought of as an energy deposition spectrum. The fraction of dose deposited by specific energy between  $z$  and  $z + dz$  is  $d(z)dz$ .<sup>b</sup> The reason for introducing the dose weighted probability density function is that the energy concentration in a site appears to determine many biological effects of radiation.

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<sup>b</sup> In order to avoid confusion with other notation involving the symbols " $f$ " and " $d$ ", probability density functions will always be written with their appropriate argument.

The more fundamental probability density functions are those due to single events. It is generally recognized that because individual events are statistically independent, a probability density function for deposition of an arbitrary dose can be constructed from the single event probability density function.<sup>1,2,3,6</sup> The remainder of section D deals with single event related quantities and their probability density functions.

Considering only single event occurrences,  $z$  represents the dose deposited in a site by a single particle. This has been denoted in previous sections by  $d$ . This is a stochastic quantity with a frequency weighted probability density function  $f_1(z)$ . The subscript "1" indicates it is associated with single events. The function  $f_1(z)$  is relevant for analyzing event numbers and frequencies resulting from irradiation of a site. The fraction of single events which occur in the site with a specific energy between  $z$  and  $z + dz$  is  $f_1(z)dz$ . The frequency mean of specific energy is given by

$$\bar{z}_F = \int_0^{\infty} z \cdot f_1(z) dz \quad (119)$$

where the subscript  $F$  is conventionally used to indicate that the average is taken using the frequency weighted probability density. This quantity is called the frequency mean specific energy per event. It is the average specific energy or average dose deposited by a single particle in the site.

Suppose a dose weighted distribution is of interest instead of a frequency weighted distribution. The fraction of dose deposited by single events with specific energy between  $z$  and  $z + dz$  is

$$d_1(z)dz = \frac{z \cdot f_1(z)dz}{\int_0^{\infty} z \cdot f_1(z)dz} \quad (120)$$

The dose weighted probability density per event is denoted by  $d_1(z)$ . It is relevant for analyzing effects of local energy concentration in an irradiated medium. The dose mean of specific energy is given by

$$\bar{z}_D = \int_0^{\infty} z \cdot d_1(z) dz \quad (121)$$

The subscript  $D$  indicates that the mean is taken using a dose weighted probability density. The quantity  $\bar{z}_D$  is called the dose mean specific energy per event. It can also be expressed in terms of  $f_1(z)$  by inserting (120) into (121).

$$\bar{z}_D = \frac{\int_0^{\infty} z^2 \cdot f_1(z) dz}{\int_0^{\infty} z \cdot f_1(z) dz} \quad (122)$$

It can now be seen that the dose mean specific energy per event is the ratio of the second moment to the first moment of specific energy per event.

$$\bar{z}_D = \frac{\bar{z}^2}{\bar{z}} \quad (123)$$

Identifying  $z$  with  $d$ , this result is equivalent to equation (37).

Table I summarizes the microdosimetry nomenclature and symbols for specific energy quantities per event, their relation to notation used in previous sections and their interpretation.

TABLE I. SPECIFIC ENERGY QUANTITIES PER EVENT

Microdosimetry Nomenclature:	Microdosimetry Symbol:	Relation to Notation in Prior Sections:	Interpretation:
specific energy	$z$	$d$	dose deposited in site by single particle
frequency mean specific energy	$\bar{z}_F$	$\bar{d}$	average dose deposited in site by single particle
dose mean specific energy	$\bar{z}_D$	$\bar{d}^2/\bar{d}$	average dose deposited in site by single particle using dose weighted probability density

### b. Specific Energy and the Two Component Model

In the Two Component Model, dose is deposited in the site as a result of direct ion strikes and as a result of secondary electrons created by ions outside of the site. The problem of describing specific energy quantities in the context of this model is related to that of a combined or mixed probability distribution. The goal is to express the overall frequency (dose) mean specific energy in terms of the frequency (dose) mean specific energies for ions and electrons.

Recall that the frequency mean specific energy is the average dose deposited in the site by a single particle. This quantity is therefore related to the ion and electron components through equation (95), the expression for the average dose of the mixed distribution of ion and electron events. Rewriting (95) in terms of microdosimetry notation,

$$\bar{z}_F = P \cdot \bar{z}_{F,ion} + (1 - P) \cdot \bar{z}_{F,e} \quad (124)$$

where  $\bar{z}_{F,ion}$  and  $\bar{z}_{F,e}$  are the frequency mean specific energies of ions and electrons, respectively. They are equivalent to the average dose deposited in the site by a single incident ion and a single

secondary electron created outside the site, respectively. Substituting the expressions for  $P$  and  $1 - P$  given by (85) and (86), the following result is obtained.

$$\bar{z}_F = \frac{\bar{N}_{ion}}{\bar{N}_{ion} + \bar{N}_e} \cdot \bar{z}_{F,ion} + \frac{\bar{N}_e}{\bar{N}_{ion} + \bar{N}_e} \cdot \bar{z}_{F,e} \quad (125)$$

The frequency mean specific energy can be expressed in terms of an ion component and an electron component, which correspond to the first and second terms in (125), respectively. The ion component is the average dose deposited by a single incident ion weighted by the fraction of ion events which occur in the site. The electron component is the average dose deposited in the site by a single electron produced in the surrounding medium by an ion, weighted by the fraction of these electron events.

Next, the dose mean specific energy per event will be written in terms of the dose mean specific energies for ions and electrons. Note that equations (37) and (123) both indicate  $\bar{z}_D$  is the ratio of the second moment to the first moment of the dose deposited by single events in the site. Equations (83) and (95) give the appropriate expressions for the second and first moments, respectively. These were obtained from Deming's general expression for the  $m^{\text{th}}$  moment of a combined or mixed distribution of alternative events given by (70). Substituting (83) and (95) into (37),

$$\bar{z}_D = \frac{P \cdot \bar{d}_{ion}^2 + (1 - P) \cdot \bar{d}_e^2}{P \cdot \bar{d}_{ion} + (1 - P) \cdot \bar{d}_e} \quad (126)$$

Solving (96) for  $P$  and (97) for  $1 - P$ , and substituting these expressions into the above equation results in

$$\bar{z}_D = f_{ion} \cdot \frac{\bar{d}_{ion}^2}{\bar{d}_{ion}} + (1 - f_{ion}) \cdot \frac{\bar{d}_e^2}{\bar{d}_e} \quad (127)$$

where  $f_{ion}$  is the fraction of dose deposited in the site by the ion component and  $1 - f_{ion}$  is the fraction of dose deposited by the electron component. Using the expressions given by (100) and (101) in the above, the final result is obtained.

$$\bar{z}_D = f_{ion} \cdot \bar{z}_{D,ion} + (1 - f_{ion}) \cdot \bar{z}_{D,e} \quad (128)$$

This result could also have been obtained by comparing equations (35) and (103). The dose mean specific energy per event can therefore be expressed in terms of an ion component and an electron component. The ion component is the dose mean specific energy for an incident ion weighted by the fraction of dose deposited in the site by ions. Similarly, the electron component is the dose mean specific energy for an electron weighted by the fraction of dose deposited in the site by electrons. Expressions for the dose mean specific energy for ions and electrons have been discussed in detail and are given by (104) and (105), respectively.

## 2. Lineal Energy Related Quantities

### a. Definition and Background

Kellerer discusses in detail the limitations of the LET concept for describing energy deposition by charged particles in small sites<sup>2,17</sup>. One problem is that transport of energy initially in the site to the outside, which results from the finite range of secondary electrons, is disregarded. Another problem is that LET is a statistical mean so that energy-loss straggling of the incident ion is not accounted for. Other limitations are also discussed in references 2 and 17. The concept of lineal energy originated to distinguish between LET, a macroscopic, average quantity, and the corresponding process which occurs in a microscopic site. The lineal energy,  $y$ , is defined<sup>6</sup> as the energy imparted to a site by one event divided by the average chord length of the site,  $\bar{c}$ .

$$y = \frac{\epsilon}{\bar{c}} \quad (129)$$

For any convex volume,  $\bar{c}$  is given by  $4V_0/S_0$  where  $V_0$  and  $S_0$  are the volume and surface area of the site, respectively. The units of  $y$  are typically keV/ $\mu\text{m}$ . As was the situation for specific energy, there are two kinds of probability density functions of interest in connection with lineal energy - frequency weighted and dose weighted.

The frequency weighted probability density function for lineal energy is denoted by  $f(y)$  and it is relevant for analyzing lineal energy event numbers and frequencies. The subscript "1" is not normally used here because it is understood that  $y$  is defined in terms of a single event. The fraction of lineal energy events with magnitude between  $y$  and  $y + dy$  is  $f(y)dy$ , and the corresponding frequency mean of lineal energy is given by

$$\bar{y}_F = \int_0^{\infty} y \cdot f(y) dy \quad (130)$$

This quantity is called the frequency mean lineal energy. Inserting (129) into (130) and transforming the  $y$  variable to  $\epsilon$  by noting that  $f(y)dy = f(\epsilon)d\epsilon$ ,

$$\bar{y}_F = \frac{\bar{\epsilon}}{c} \quad (131)$$

The quantity  $\bar{y}_F$  is similar to LET, assuming that the particle loses only a small fraction of its energy in the site and that escape of secondary electrons from the site can be neglected.

Suppose the effects of local energy concentration in the medium are of interest. Then the dose weighted distribution of lineal energy,  $d(y)$ , is used. Since  $y$  is proportional to the dose deposited in the site by a single event, the fraction of dose deposited by lineal energy between  $y$  and  $y + dy$  is

$$d(y)dy = \frac{y \cdot f(y)dy}{\int_0^{\infty} y \cdot f(y)dy} \quad (132)$$

The corresponding dose mean of lineal energy is given by

$$\bar{y}_D = \int_0^{\infty} y \cdot d(y)dy \quad (133)$$

This quantity is called the dose mean lineal energy. Its relation to the frequency weighted probability density function,  $f(y)$ , is seen by substituting equation (132) into (133).

$$\bar{y}_D = \frac{\int_0^{\infty} y^2 \cdot f(y) dy}{\int_0^{\infty} y \cdot f(y) dy} \quad (134)$$

Equation (134) shows that the dose mean lineal energy is the ratio of the second moment to the first moment of the lineal energy distribution in the site.

$$\bar{y}_D = \frac{\overline{y^2}}{\bar{y}} \quad (135)$$

It will be recalled that equation (123) is a similar relation for the dose mean specific energy per event.

Substituting (129) into (134) and transforming the integration variable to  $\epsilon$ , the result can also be expressed as

$$\bar{y}_D = \frac{1}{c} \cdot \frac{\overline{\epsilon^2}}{\bar{\epsilon}} \quad (136)$$

Table II summarizes the microdosimetry nomenclature and symbols for lineal energy related quantities, their relation to notation used in previous sections and their interpretation.

TABLE II. LINEAL ENERGY QUANTITIES

Microdosimetry Nomenclature:	Microdosimetry Symbol:	Relation to Notation in Prior Sections:	Interpretation:
lineal energy	$y$	$\epsilon/\bar{c}$	energy deposited in site by single particle divided by average chord length of site
frequency mean lineal energy	$\bar{y}_F$	$\bar{\epsilon}/\bar{c}$	average energy deposited in site divided by average chord length of site
dose mean lineal energy	$\bar{y}_D$	$\overline{\epsilon^2}/(\bar{\epsilon}\cdot\bar{c})$	average lineal energy deposited in site using dose weighted probability density

### b. Lineal Energy and the Two Component Model

First an expression for the frequency mean lineal energy will be obtained in terms of the frequency mean lineal energies for ions and electrons. Recall from equation (131) that  $\bar{y}_F$  is the average energy deposited in the site by a single particle divided by the average chord length of the site. In the Two Component Model, the average energy deposited by an ion event is

$$\overline{\epsilon}_{ion} = f_{ion} \cdot \overline{L}_{ion} \cdot \overline{s}_{ion} \quad (137)$$

where  $L_{ion}$  is the ion's unrestricted LET. Assuming that tertiary electrons generated within the site by incident secondary electrons are not energetic enough to escape the site, the average energy deposited by an electron event is

$$\overline{\varepsilon_e} = \overline{L_e} \cdot \overline{s_e} \quad (138)$$

where  $L_e$  is the unrestricted LET of the incident electron.

From considerations similar to those applied to equations (124) and (125) in the previous section, equation (131) can be rewritten as

$$\overline{y_F} = \frac{\overline{N_{ion}}}{\overline{N_{ion}} + \overline{N_e}} \cdot \frac{\overline{\varepsilon_{ion}}}{c} + \frac{\overline{N_e}}{\overline{N_{ion}} + \overline{N_e}} \cdot \frac{\overline{\varepsilon_e}}{c} \quad (139)$$

In analogy to equation (131), the frequency mean lineal energy for ions and electrons can be identified as

$$\overline{y_{F,ion}} = \frac{\overline{\varepsilon_{ion}}}{c} \quad (140)$$

and

$$\overline{y_{F,e}} = \frac{\overline{\varepsilon_e}}{c} \quad (141)$$

Then (139) can be rewritten

$$\overline{y_F} = \frac{\overline{N_{ion}}}{\overline{N_{ion}} + \overline{N_e}} \cdot \overline{y_{F,ion}} + \frac{\overline{N_e}}{\overline{N_{ion}} + \overline{N_e}} \cdot \overline{y_{F,e}} \quad (142)$$

Equations (140), (141) and (142) are used to evaluate the frequency mean lineal energy in the Two Component Model.

Due to the similarity of the quantities  $\overline{z_F}$  and  $\overline{y_F}$ , it is worthwhile at this point to write

down the exact relations for these quantities and for their components. Comparing the interpretation of  $\bar{z}_F$  given in table I with the expression for  $\bar{y}_F$  given by equation (131), it is seen that

$$\bar{z}_F = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \bar{c} \cdot \bar{y}_F \quad (143)$$

In this expression,  $\bar{z}_F$  is in rads,  $\bar{y}_F$  in keV/ $\mu\text{m}$ ,  $\bar{c}$  in  $\mu\text{m}$ ,  $V_0$  in  $\text{cm}^3$  and  $\rho_0$  in  $\text{g}/\text{cm}^3$ . Similar relations exist for both ion events and electron events.

$$\bar{z}_{F,ion} = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \bar{c} \cdot \bar{y}_{F,ion} \quad (144)$$

and

$$\bar{z}_{F,e} = \frac{1.6 \times 10^{-11}}{V_0 \cdot \rho_0} \cdot \bar{c} \cdot \bar{y}_{F,e} \quad (145)$$

Finally, an expression for the dose mean lineal energy will be obtained in terms of the dose mean lineal energies of ions and electrons. Comparing equations (36) and (136), it can be seen that a relation analogous to equation (143) exists for the dose weighted quantities  $\bar{z}_D$  and  $\bar{y}_D$ .

$$\bar{y}_D = \frac{V_0 \cdot \rho_0}{1.6 \times 10^{-11}} \cdot \frac{1}{\bar{c}} \cdot \bar{z}_D \quad (146)$$

Substituting (128) into the above expression gives  $\bar{y}_D$  in terms of the two components.

$$\bar{y}_D = \frac{V_0 \cdot \rho_0}{1.6 \times 10^{-11}} \cdot \frac{1}{\bar{c}} \cdot [f_{ion} \cdot \bar{z}_{D,ion} + (1 - f_{ion}) \cdot \bar{z}_{D,e}] \quad (147)$$

The dose mean lineal energy can therefore be written

$$\overline{y_D} = f_{ion} \cdot \overline{y_{D,ion}} + (1 - f_{ion}) \cdot \overline{y_{D,e}} \quad (148)$$

where

$$\overline{y_{D,ion}} = \frac{V_0 \cdot \rho_0}{1.6 \times 10^{-11}} \cdot \frac{1}{c} \cdot \overline{z_{D,ion}} \quad (149)$$

and

$$\overline{y_{D,e}} = \frac{V_0 \cdot \rho_0}{1.6 \times 10^{-11}} \cdot \frac{1}{c} \cdot \overline{z_{D,e}} \quad (150)$$

Note that these last two relations can be obtained by applying equation (146) to the appropriate type of event.

In order to put the last two expressions in a form more amenable to calculations, they will be rewritten in terms of the appropriate random physical variables. Inserting equation (104) into (149) gives the result

$$\overline{y_{D,ion}} = \frac{1}{c} \cdot \left( f_{ion} \frac{\overline{L_{ion}^2}}{\overline{L_{ion}}} \cdot \frac{\overline{s_{ion}^2}}{\overline{s_{ion}}} + \frac{\overline{\delta_{ion}^2}}{\overline{\delta_{ion}}} + F_{ion} \cdot \overline{w_{ion}} \right) \quad (151)$$

Similarly, substituting equation (105) into (150) results in

$$\overline{y_{D,e}} = \frac{1}{c} \cdot \left( \frac{\overline{L_e^2}}{\overline{L_e}} \cdot \frac{\overline{s_e^2}}{\overline{s_e}} + \frac{\overline{\delta_e^2}}{\overline{\delta_e}} + F_e \cdot \overline{w_e} \right) \quad (152)$$

A summary of the quantities on the right-hand side of equations (151) and (152) is given in section C2 immediately after equation (105). Equations (148), (151) and (152) are used to evaluate the dose mean lineal energy in the Two Component Model.

## E. Overview

This section provides an overview of the ideas involved in the Two Component Model, which have been discussed in section II. This will be accomplished with the aid of flow charts. The chart in figure 4 indicates the applied probability methods used to combine the appropriate random variables and variances. The sequence of operations begins with the random variables displayed on the left side of the figure and ultimately leads to the variance of the total energy deposited in the site. Factors unimportant to the overview such as conversions between energy and dose and conversions between variances and relative variances are not included in the figure.

First of all, the fluctuations in energy deposited in the site by a single particle are considered. The fluctuations depend on the product of the random variables due to LET and path length. As shown on the left hand side of the chart, this applies separately to ion events and to electron events. Combining  $L_{ion}$  with  $s_{ion}$  and  $L_e$  with  $s_e$  results in the two indicated variances. (To simplify the notation in the chart, the usual subscripts "ion" and "e" are not included with the already subscripted "L" and "s" variables. Whether the variance refers to ions or electrons is clear from the argument. Similar reasoning applies to the other variances in the column of six variances.) The appropriate expressions for these two variances are obtained by applying equation (40) to ions and electrons, respectively. The key equation numbers are indicated at the appropriate points in the flow chart. Next, energy-loss straggling is considered. The variables  $n$  and  $\delta$  are combined making use of Burgess' variance theorem and that result is modified using the fact that  $n$  is controlled by Poisson statistics. Again, this is done for both ions and electrons, and the resultant variances for straggling are obtained by applying equation (44) to ion events and to electron events. If ionization fluctuations rather than energy fluctuations are of interest, then the random variables  $\eta_{ion}$  and  $\eta_e$  must be considered in addition to the variables mentioned above. These two random variables are combined with their associated Fano factor to give the variances due to Fano fluctuations. Expressions for the last two variances are obtained by applying equation (50) to the two situations. Proceeding to the right in the figure past the first six boxes which correspond to the six operations discussed above, note there are six resulting variances. Three contribute to the total variance of a single ion event while the other three contribute to the total variance of a single electron event in the site.

The three variances associated with the ion component are considered to be the result of "simultaneous events" of the type discussed in section C1. They are therefore summed to give the total variance due to single ion events,  $var(\epsilon_{ion})$ . The expression for this variance is obtained from the application of equation (51) to an ion event. In a similar manner, the three variances due to electron events are summed to give the total variance due to single electron events,  $var(\epsilon_e)$ .

The next step is to combine the previous single event variances with the corresponding random number of events. This is done with Burgess' variance theorem. Then, assuming the event numbers are subject to Poisson statistics, the expressions for the variance of the total energy deposited by ions,  $var(E_{ion})$ , and the variance of the total energy deposited by electrons,

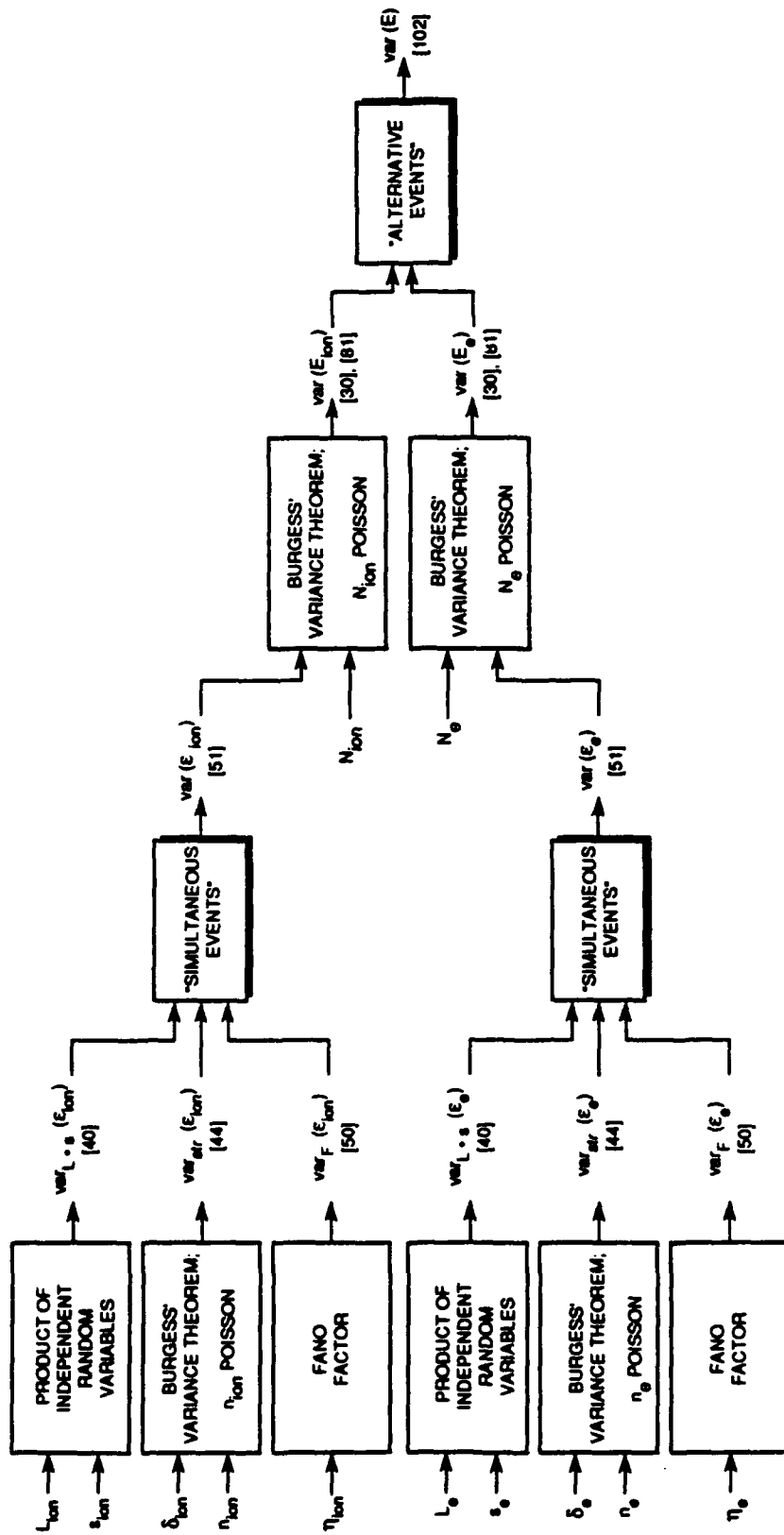


Figure 4. Overview of the combination of the appropriate quantities in the Two Component Model to obtain the expression for the variance of the total energy deposited in the site.

$var(E_e)$ , are obtained. The corresponding expressions result from applying either (30) or (81) to the appropriate event type. Up to this point, the energy deposition by ions and electrons have been considered separately.

The last step is to combine the variance of the energy deposition distribution due to ions with that due to electrons. The two distributions are treated as "alternative event" distributions of the type discussed in section C1. The final result is the variance of the total energy deposited in the site and is given by equation (102).

A brief overview of the construction of the microdosimetric quantities  $\bar{z}_F$ ,  $\bar{z}_D$ ,  $\bar{y}_F$  and  $\bar{y}_D$  in the context of the Two Component Model will now be given as a conclusion to this section. Two schemes are indicated within the flow chart displayed in figure 5. The upper scheme shows an overview of the two frequency averaged quantities while the lower scheme shows the two dose averaged quantities.

First, the frequency averaged quantities will be considered. To obtain the frequency mean specific energy per event,  $\bar{z}_F$ , the first moments of the quantities  $z_{F,ion}$  and  $z_{F,e}$  are combined using the results of alternative event distributions. The result is given by equation (125). This is equivalent to calculating the average dose deposited by the mixed distribution of ion and electron events.

Recall that specific energy and lineal energy are the microscopic analogues of dose and LET, and are related to each other through equation (143). As indicated in figure 5, the final expression for the frequency mean lineal energy,  $\bar{y}_F$ , can be obtained by relating  $\bar{z}_F$  to  $\bar{y}_F$  and incorporating the average chord length of the target site. The final result is equation (142).

Finally, the dose averaged microdosimetric quantities are considered. To obtain the expression for  $\bar{z}_D$ , which contains the information describing the single particle variability of deposited dose, the combination of random variables proceeds as indicated in figure 4 up to the expressions for  $var(e_{ion})$  and  $var(e_e)$ . At this point some algebraic manipulations will convert these two variances to the expressions for the dose mean specific energy per ion event, given by (104), and the corresponding quantity for electron events, given by (105). These two quantities are then combined using the results for alternative event distributions to obtain  $\bar{z}_D$ , equation (128). The expression for the dose mean lineal energy,  $\bar{y}_D$ , can then be obtained by relating  $\bar{z}_D$  to  $\bar{y}_D$  which involves incorporating the average chord length of the target site. The final result is equation (148).

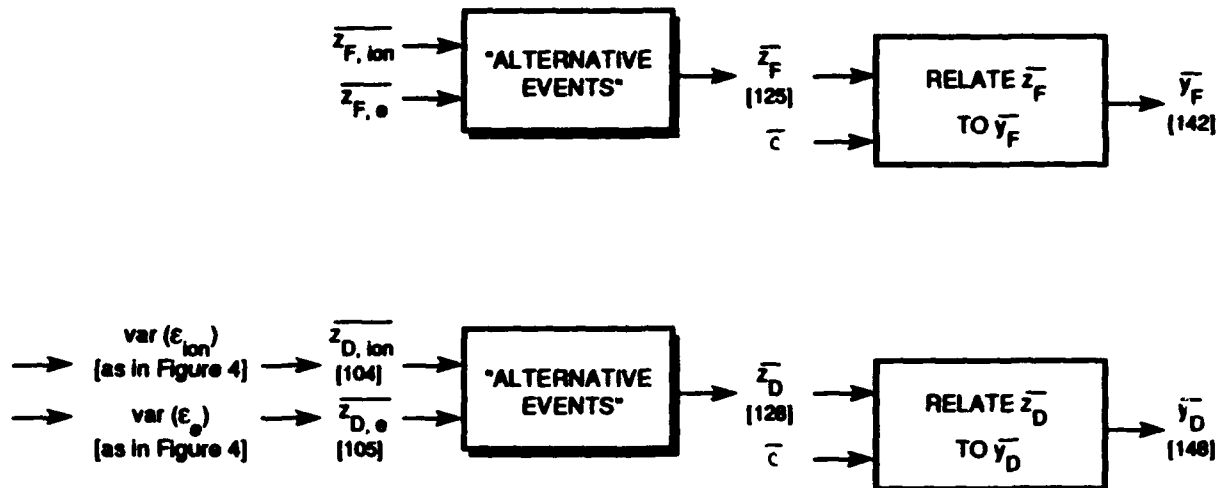


Figure 5. Overview of the combination of the appropriate quantities in the Two Component Model to obtain expressions for the indicated microdosimetric quantities.

### III. SUMMARY

The basic equations of the Two Component Model have been derived in detail beginning with well known concepts in stochastic theory. The model is a first principles, analytic description of energy deposition fluctuations in ion-irradiated sites which may be as small as nanometers. The new and key feature of the model is based on combining the dose distributions which result from two types of single events that occur in the irradiated site. The first is a direct ion interaction with the site. The second is a secondary electron interaction with the site, the electron having been produced by an ion in the surrounding medium. General expressions for the frequency mean and dose mean specific energy per event and for the frequency mean and dose mean lineal energy have also been obtained in terms of the two components. All of the derived results are applicable to a wide variety of conditions, which include different types of ions, and different target site dimensions, geometries and materials. The model can be used to calculate both the energy deposition and the electron-hole pair production fluctuations in the site. These are all important considerations for both experimental and theoretical investigations of small sites irradiated with ions, and has direct implications for radiation effects in biological systems and modern microelectronics.

The next report will discuss how the basic equations and quantities are evaluated and how these results compare with other published calculations based on Monte Carlo techniques.

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