Track Structure

The initial spatial pattern of energy deposition by ionizing radiation plays a significant role in the subsequent evolution of biologically active chemical species. Radiochemical and radiobiological models of radiation action initiated by high linear energy transfer (LET) particles rely heavily on an accurate description of charged particle tracks. Our study of track structure includes both theoretical and experimental investigation of the spatial pattern of energy deposition. Incorporation of these data into models of energy transport in condensed phase clarifies the effects of the initial spatial patterns on evolving chemical yields. Because of the experimental limitations on determination of energy deposition in nanometer-sized volumes, we have continued to develop Monte Carlo codes to calculate ionization and energy imparted in small sites. During the past year, we extended our study of the systematics of energy deposition in small sites to include energy deposition by ions just outside the volume of interest and completed our characterization of those events produced by ions that cross the site. The Monte Carlo codes were also extended for calculation of energy deposition by heavy (HZE) particles to begin to provide stochastic information of interest to the radiation biology of high-energy heavy ions. The modeling of stochastic processes in the transfer of energy in macromolecular systems focused on understanding anisotropic radical yields observed in neutron irradiation of oriented deoxyribonucleic acid (DNA) fibers. These studies have benefited from close collaboration with other researchers around the world, including H. G. Paretzke, GSF Institute für Strahlenschutz, Neuherberg, West Germany; D. E. Charlton, Concordia University, Canada; J. J. Coyne, National Bureau of Standards (NBS); L. S. Myers and C. Swenberg, Armed Forces Radiobiology Research Institute (AFRRI), Bethesda, Maryland; T. L. Criswell, Boeing Aerospace Company, Seattle, Washington; and D. Goodhead, Medical Research Council (MRC), Harwell, England.

APPLICATION OF TRACK STRUCTURE IN MICRODOSIMETRY

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A paper on proton ionization and energy deposition in submicron sites, entitled "Microdosimetric Aspects of 0.3 to 20 MeV Proton Tracks: I. Crossers" has been prepared for submission to Radiation Research; the abstract is presented here.

Comprehensive results are presented for the evaluation of microdosimetric quantities from track structures of fast protons obtained by computer simulation using a detailed-history Monte Carlo method. Stochastic frequency distributions for energy imparted and number of ionizations were calculated for 0.3 to 20 MeV protons passing through spherical sites of 2 nm to 1 μm diameter in unit-density water. From these the dependencies of the first two moments of the distributions on ion energy, site size, and position of the track within the site were derived. The frequency distributions are fitted in the least-squares sense by simple analytic (lognormal) functions to facilitate their use in further microdosimetric considerations.

AN ANALYTIC MODEL FOR IONIZATION DISTRIBUTIONS PRODUCED IN NANOMETER SITES BY PROTONS

W. E. Wilson and H. G. Paretzke

Extensive computer simulations of proton tracks have been made for protons of energy E, passing through spherical sites of diameter d, off center by a distance b, which we call eccentricity. Computed ionization distributions for $0.3 < E < 20$ MeV, $2 < d < 1000$ nm, and $0 < b < d/2$ were obtained. The lognormal function,

$$f(j) = \mathrm{EXP}(-\ (\ln(j)-\mu)^2\ /\ 2\,\sigma^2\ )\ /\ \sigma\ j\ (2\pi) \qquad (1)$$

is used to represent these distributions phenomenologically. To achieve this representation the function was fitted in the least-squares sense to the ionization distributions, thus providing the dependence of the two parameters μ and σ on E, d, and b. The dependence of μ on E and d is rather simple; μ can be described mathematically by the expression

$$\mu = c_1\log_{10}(d) + c_2\log_{10}(E) + c_3(b) \qquad (2)$$

where c_1 and c_2 are independent of eccentricity and c_3 is independent of both E and d. The values of $c_1 = 2.55817$ and $c_2 = -2.06716$ were obtained by multiple-linear regression of equation (2) to the μ versus E versus d data, and c_3 is given by

$$c_3 = 10.\ (0.45 - 0.5056\ (1-b^2)^{1/2}) \quad (3)$$

The width parameter σ is obtained from the ratio of the variance, V, to the mean, $< j >$, of the distributions in ionization. This ratio is essentially independent of ion energy E up to a given diameter, at which point the ratio saturates. The size of this diameter depends on ion energy because, as the diameter is increased, the site eventually becomes large enough to contain the most energetic delta-ray for that ion energy; i.e., all deltas become stoppers.

We have approximated the behavior of the ratio, $V/<J>$, by

$$(V/<J>) = d^{0.556} \quad (4)$$

and the saturation value by

$$(V/<j>_{max}) = 1385.\ E/\ln(69.1\ E) \quad (5)$$

It can be shown that, for the lognormal distribution,

$$<j> = EXP(\mu + \sigma^2/2) \quad (6)$$

and

$$V = (EXP(\sigma^2) - 1)\ EXP(2\ \mu + \sigma^2) \quad (7)$$

These two equations can be combined and reduced to

$$g(\sigma^2) = \sigma^2/2 + \ln(EXP(\sigma^2) - 1) + \mu - \ln(R) = 0 \quad (8)$$

where $R = V/<J>$.

The width parameter σ is obtained by numerically solving for the zero of equation (8). A concise computer code system written in FORTRAN is under development to evaluate this model of the stochastics of ionization.

For high-velocity charged particles and sufficiently small sites it is quite possible for the particle to pass through the site without depositing any energy or without ionization. This situation indicates a breakdown in the proportionality between fluence and dose, and it is therefore desirable to know how frequently this happens and, ideally, to be able to quantify the frequency. From the computer simulations it was discovered that in sites smaller than 1000 nm in diameter, the frequency for zero ionization is simply related to the cross section for ionization,

$$f(j\text{-}0) = EXP\ [\ - \frac{d\ (1 - b^2)^{1/2}}{\lambda_j(E)_p}\ ] \quad (9)$$

where j is the ionization number and λ_j is the mean free path for the interaction. The numerator of the exponential argument in equation (9) is just the path length of the ion through the site when it has a relative eccentricity of b. Equation (9) gives an upper limit for the frequency for zero interaction, because ionization produced by secondary electrons should sometimes be a contributing factor and thereby reduce the frequency for zero interaction. That this does happen has been confirmed by the simulations.

MICROSCOPIC DOSIMETRY OF IONS IN NANOMETER SITES: TOUCHERS

W. E. Wilson and H. G. Paretzke

Two types of events are of primary importance in the submicron dosimetry of fast protons. The foremost are those events caused by protons that pass through the site, and therefore called "crossers." Second are events caused by protons that pass outside the site but that deposit energy via secondary electrons (delta-rays) that do enter the site. Such events have been called "touchers" in the literature.

As part of our continuing study of the systematics of proton track structure, we are computing the ionization and energy deposition distributions for toucher events for 0.3 to 20 MeV protons and sites from 10 to 200 nm as a function of radial distance (eccentricity) from the proton path. Results to date,