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OPENING OF THE SYMPOSIUM

G.W. BARENSEN  
(invited paper)                      The Importance of Microdosimetry  
for Radiation Biology and Radia-  
tion Protection.

SESSION I

Chairman : Mr. FOWLER

H.H. ROSSI  
(invited paper)                      Microscopic Distribution of  
Radiation Energy.

A.M. KELLERER                      Calculation of Energy Deposition  
Spectra.

K. WILSON  
E.W. EMERY                          Path Length Distributions Within  
Cylinders of Various Proportions.

SESSION II

Chairman : Mr. ROSSI

J.F. FOWLER  
(invited paper)                      Biological Significance of Shape  
and Volume of Microdosimeters.

J. BOOZ  
Th. SMIT                              Development of a Chromosome  
Counter.

S.B. FIELD  
K. WILSON                              Some Measurements with a ROSSI  
Tissue Equivalent Proportional  
Counter.

J.S. BEVAN                          Microdosimetry in Cylindrical  
Volumes : Interim Report on a  
Project Using a Tissue Equivalent  
Proportional Counter.

W.A. GLASS                          Interaction of Low Energy Protons  
with Thin Layers of Tissue-like  
Material

SESSION III

Chairman : Mr. ALLISY

G.J. NEARY  
(invited paper)

The Dependence of the Biological Effectiveness of Radiation on Physical Factors of Radiation Quality, and the Significance of such Dependence.

G.W. BARENSEN

Relative Biological Effectiveness as a Function of Linear Energy Transfer.

J.W. BAUM  
S.L. STONE  
A.V. KUEHNERRadial Distribution of Dose Along Heavy Ion Tracks,  $LET_r$ .

A.H. SULLIVAN

The Estimation of the Local Energy Loss Distribution of Ionizing Radiation from Observations of Ion Recombination in a Gas.

J.A. DENNIS

The Application of JAFFÉ and LEA Theories of Recombination to the Determination of LET and QF with Ionization Chambers.

J. BOOZ

The Relation Between Energy Absorption and Ionization in Tissue Equivalent Gas for Gamma Quants of Low Energy.

SESSION IV

Chairman : Mr. POHLIT

J.J. BROERSE  
G.W. BARENSEN

The Importance of Secondary Particle Equilibrium for Neutron Irradiations of Cultured Cells and Intact Organisms.

D. HARDER  
H.J. SCHULZ

Buildup and Equilibrium of Secondary Electrons for High-Energy Electron Radiation.

H.A. WRIGHT

Calculation of the Buildup of Dose in Tissue Irradiated by High Energy Neutrons and Protons.

VII

SESSION V

Chairman : Mr. BARENSEN

D.E. CHARLTON  
D.V. CORMACK

A Comparison of Models of Electron Liberation and Passage Through Matter Used in Calculating Absorbed Dose near an Irradiated Interface.

G. DREXLER

Verlauf der Ionendosis an Grenzschichten.

T.E. BURLIN  
F.K. CHAN

The Influence of Interfaces on Dosimeter Response.

T.E. BURLIN  
B.W. HANCOCK

The Vacuum Chamber as an Interface Dosimeter.

SESSION VI

Chairman : Mr. HARDER

F.W. SPIERS  
(invited paper)

Dosimetry at Interfaces with Special Reference to Bone.

P.J. DARLEY

Measurement of Linear Path Length Distributions in Bone and Bone Marrow Using a Scanning Technique.

G.D. ZANELLI

Thermoluminescence Methods Applied to Dosimetry in Trabecular Bone.

SESSION VII

Chairman : Mr. BLANC

W. SENGPIEL  
J. BOOZ

Energy Transfer of Alpha Emitters to the Soft Tissue in Cylindrical Bone Cavities.

A.D. KAPPOS

Energieabsorptionsspektren bei Inkorporation alpha-strahlender Nuklide.

W. KÜHN

Methode zur Berechnung der Dosis bei inkorporierten Beta-Strahlern in annähernd symmetrischen Mikrobereichen.

A. WAMBERSIE  
J. DUTREIX

L'Utilisation des Dosimètres Biologiques pour la Détermination des Doses aux Interfaces.

SESSION VIII

Chairman : Mr. SPIERS

J. KASTNER  
 B.A. CAMERON  
 M.A. PAESLER  
 R.K. LANGS

New Developments in Photolumi-  
 nescent Microdosimeter Measure-  
 ment.

K.H. CHADWICK  
 W.F. OOSTERHEERT

Radiation Induced Thermolumi-  
 nescence of Tomato Seeds at  
 Low Temperature.

R.J. SCHULZ

Interface Dosimetry with LiF-  
 Teflon Microdosimeters.

G.M. SCHMIDT-BURBACH

Untersuchungen zur Dosimetrie  
 an punktförmigen radioaktiven  
 Teilchen.

SESSION IX

Chairman : Mr. NEARY

D. BLANC  
 J. MATHIEU  
 J.P. PATAU

Détermination Théorique des  
 Transferts d'Energie Linéique  
 des Rayonnements dans certains  
 Diélectriques Liquides.  
 Mesures Expérimentales.

B.A. ENGELKE  
 W. OETZMANN

Influence of Thin Air-Equi-  
 valent Layers on the Pressure  
 Dependence of the Mean Ion  
 Dose Rate.

H. JOFFRE  
 L. PAGES

Relations Fondamentales entre  
 Transfert Linéique d'Energie,  
 Dose Absorbée, Kerma et Exposi-  
 tion. Application aux Change-  
 ments de Milieux.

G.J. NEARY

Closing Remarks.

List of Participants

## AUTHORS INDEX

BARENSEN, G.W. 1 - 249 - 353	KASTNER, J. 621
BAUM, J.W. 269	KELLENER, A.M. 57
BEVAN, J.S. 161	KUEHNER, A.V. 269
BLANC, D. 681	KÜHN, W. 583
BOOZ, J. 125 - 331 - 551	LANGS, R.K. 621
BROERSE, J.J. 353	MATHIEU, J. 681
BURLIN, T.E. 447 - 461	NEARY, G.J. 205 - 777
CAMERON, B.A. 621	OETZMANN, W. 719
CHADWICK, K.H. 633	OOSTERHEERT, W.F. 633
CHAN, F.K. 447	PAESLER, M.A. 621
CHARLTON, D.E. 413	PAGES, L. 733
CORMACK, D.V. 413	PATAU, J.P. 681
DARLEY, P.J. 509	ROSSI, H.H. 27
DENNIS, J.A. 313	SENGPIEL, W. 551
DREXLER, G. 433	SCHMIDT-BURBACH, G.M. 689
DUTREIX, J. 603	SCHULZ, H.J. 385 - 643
EMERY, E.W. 79	SMIT, Th. 125
ENGELKE, B.A. 719	SPIERS, F.W. 473
FIELD, S.B. 147	STONE, S.L. 269
FOWLER, J.F. 93	SULLIVAN, A.H. 295
GLASS, W.A. 189	WAMBERSIE, A. 603
HANCOCK, B.W. 461	WILSON, K. 79 - 147
HARDER, D. 385	WRIGHT, H.A. 409
JOFFRE, H. 733	ZANELLI, G.D. 527
KAPPOS, A.D. 569	Liste des participants 781

## CALCULATION OF ENERGY DEPOSITION SPECTRA

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**Abstract:** Classical straggling theory is of limited applicability in microdosimetry. A new derivation of the energy loss distributions and some theoretical properties of the Compound Poisson process are discussed.

The energy transfer from an ionizing particle to a structure of microscopic dimensions is a stochastic process. Rigorous treatment of this highly complicated process has become possible since ROSSI and co-workers<sup>1</sup> have introduced the spectra,  $P(\Delta Z)$ , of local energy increments. It is the strength of ROSSI's concept that, unlike classical LET-theory, it integrates all the different factors involved. Therefore, it covers efficiently even those cases which are still too complex to be understood in all details. With the steadily improving experimental determination of the local energy density spectra, however, with their increasing impact on radiation biology, and with the emergence of a theory of microdosimetry one has to look for the complete picture. It turns out that the local energy density spectra are far more than a mere synthesis of LET-spectra and track length distribution in the sensitive structures. The statistical nature of energy deposition along the track of an ionizing particle is a most important additional aspect brought up by microdosimetry (if we may use this somewhat preposterous name for the moment). In many instances it is also the decisive factor for the shape of the local energy density spectra. Track length distribution and even LET-spectra are often of minor importance<sup>2</sup>.

Even in those cases where 'straggling' is not the decisive factor, it is still the one which presents the most serious difficulties as far as physical knowledge and mathematical evaluation

are concerned. One may almost state that calculation of local energy density spectra is essentially a problem of computing the energy loss distributions. If this problem is solved the explicit probability distributions for different sizes of the critical area and for different LET-spectra are put together easily. This may be seen from first calculations which some years ago have been done in a Monte Carlo approximation<sup>3</sup>.

This paper is concerned with the derivation of the energy loss distributions for an additional reason. In radiation physics the problem of energy straggling has been treated extensively. The theories of BOHR<sup>4</sup>, LANDAU<sup>5</sup>, and SYMON<sup>6</sup> have led to the recent solution given by VAVILOV<sup>7</sup>, and to its tabulation by SELTZER and BERGER<sup>8</sup>. This solution is based on a few simplifying assumptions. It neglects the atomic binding of the electrons, and while, on the one hand, it requires that only a minor fraction of the kinetic energy of the ionizing particle is lost, it is, on the other hand, restricted to a large number of primary collisions. These approximations, while perfectly valid in some high energy applications, turn out to be prohibitive in microdosimetry. In radiobiological applications the binding energy of the electrons cannot be neglected, the number of collisions in the structures of interest is often small, and a delta-ray cut-off has to be applied whenever only the energy locally imparted is of interest.

For these reasons a new method has been developed for the derivation of the energy loss distributions for arbitrary collision laws over the whole range of collision numbers. While this approach may be the only choice in many radiobiological applications, it should also prove useful in general radiation physics and even in high energy physics, whenever more rigorous treatment - for example, a correction for delta-ray escape in the work with solid state detectors (see <sup>9</sup>) - is desired.



## I. Derivation of the energy loss distributions

Let us for the moment assume that the collision law, or delta-ray spectrum, is known. Let us also restrict our discussion to a constant value of the stopping power, i. e. to the case of an ionizing particle which in traversing a certain distance loses only a small fraction of its kinetic energy. For easier understanding some reference will be given to the VAVILOV-theory, and also the notation will be kept similar to the one which is used, for example, in the NAS report on the penetration of charged particles in matter<sup>10</sup>. We will, however, not use that part of the conventional terminology which is merely connected with the special solutions valid for the  $1/E^2$  collision law or its relativistic modification.

Let  $f(E,s) \cdot dE$  denote the probability that an ionizing particle in traversing a path length  $s$  in the target will suffer an energy loss between  $E$  and  $dE$  as the result of successive collisions with atomic electrons. The energy loss  $E$  in the target may vary over a wide range. The fluctuations are due to the varying number of collisions in the target, and, what is much more important, to the varying amount of energy transferred in the individual collisions. If the single collision spectrum is designated by  $c(E)$ , then  $c(E) \cdot dE$  is the probability that a single collision leads to an energy transfer between  $E$  and  $dE$ .

VAVILOV has derived the distributions  $f(E,s)$  by integrating the transport equation:

$$\frac{\partial f(E,s)}{\partial s} = k \cdot \left( \int_{e_{\min}}^b f(E-x,s) \cdot c(x) dx - f(E,s) \right) \quad (1)$$

By use of the Laplace transform he derives solutions for the  $1/E^2$  collision law and its relativistic modifications. The disadvantage of the method is that it cannot be used for modified collision spectra which take into account the electron binding and the escape and influx of delta rays. Moreover the solutions are expressed as an integral over some complicated functions. This has made it necessary to adopt a mixed analytical numerical procedure<sup>8</sup>.

A direct and generally applicable numerical method avoids these disadvantages. The alternative method derives the energy loss distributions from an integral equation which is characteristic for the Compound Poisson process. This integral equation expresses the fact that the energy loss in neighbouring track segments is statistically independent:

$$f(E, s_1 + s_2) = \int_0^E f(E-x, s_1) \cdot f(x, s_2) dx \quad (2)$$

This means that, if a distance is split up into two parts, its energy loss distribution is the convolution of the two distributions belonging to the individual parts. Specifically we may choose two equal segments, and obtain:

$$f(E, 2s) = \int_0^E f(E-x, s) \cdot f(x, s) dx \quad (3)$$

Repeated application of this formula leads to arbitrarily high values of  $s$ . If, therefore, the energy loss distribution is known for a thin target it can be derived for all other values of  $s$ .

An essential point is that with repeated convolutions the increase in mean energy loss is exponential. Only 10 successive convolutions are necessary to span a factor of  $2^{10}$ , i. e. to reach approximately 1000 times the original target size. This can be made clear by the following equations where a star is used as a shorthand notation for the convolution process:

$$\begin{aligned} f(E, 2s) &= f(E, s) * f(E, s) \\ f(E, 4s) &= f(E, 2s) * f(E, 2s) \\ f(E, 8s) &= f(E, 4s) * f(E, 4s) \end{aligned} \tag{4}$$

$$f(E, 2^n \cdot s) = f(E, 2^{n-1} \cdot s) * f(E, 2^{n-1} \cdot s)$$

All we need, therefore, is the energy loss distributions for very small distances. These, however, can be given easily. If the distance  $s$  is so small that in most cases no collision at all occurs, then the probability for more than one collision can be neglected and the distribution of energy loss is a simple superposition of a delta function at zero energy and the single collision spectrum  $c(E)$ :

$$f(E, s) = (1-\epsilon) \cdot \delta(E) + \epsilon \cdot c(E) \tag{5}$$

where  $\epsilon \ll 1$  is the mean collision number.

If, for example, we start with  $\epsilon = 2^{-10}$ , then the probability for more than one collision is equal to  $2^{-20}$  and can be safely neglected. By 20 successive convolutions one generates a set of energy loss distributions of which the last one belongs to a mean collision number of 1012. By choosing the appropriate starting point  $s$ , one can reach any desired mean energy loss.

This is in short summary the principle of the derivations of the energy loss distributions. It gives enough information to use the computer program developed on this basis. Nothing more is required than the read-in of the single collision law  $c(E)$  and the values of mean energy loss for which the distribution functions are desired.

Nevertheless, it may be useful to mention at least some details of the actual procedure. This will be done in the next paragraph which is of more technical nature and may, therefore, be used in conjunction with the program itself.

First, however, some remarks on the moments of the energy loss distribution should be inserted. Theoretical determination of the moments and comparison with the numerically obtained values can be used for the accuracy control of the computations.

It can be shown, though a proof will not be given here, that certain combinations of the moments, the so-called semi-invariants of the distribution  $f(E,s)$ , all increase linearly with  $s$ . Also their dependence on the moments of the collision spectrum  $c(E)$  is simple. Let us designate the non-central moments of  $c(E)$  by  $c_n$ :

$$c_n = \int_0^{e_{\max}} E^n \cdot c(E) dE \quad (7)$$

Then one may derive that the  $n$ -th semiinvariant of the energy loss distribution is equal to the  $n$ -th non-central moment of the collision spectrum times the mean collision number. The second and the third semiinvariant are equal to the second and the third central moment, and the fourth semiinvariant is equal to the fourth central moment minus 3 times the variance. Thus

one obtains the following formulas for the central moments of the energy loss distribution:

$$\begin{aligned}
 \bar{E} &= N \cdot c_1 && (N \text{ is the mean collision number}) \\
 \overline{(E-\bar{E})^2} &= N \cdot c_2 = \bar{E} \cdot c_2 / c_1 \\
 \overline{(E-\bar{E})^3} &= N \cdot c_3 = \bar{E} \cdot c_3 / c_1 \\
 \overline{(E-\bar{E})^4} &= N \cdot c_4 - 3(N \cdot c_2)^2 = \bar{E} \cdot c_3 / c_1 - 3(\bar{E} \cdot c_2 / c_1)^2
 \end{aligned}
 \tag{8}$$

These are important general properties of the Compound Poisson process.

It should be noted that the higher moments depend strongly on the tails of the distributions. These tails can be computed accurately, but they cannot in general be determined exactly in the experiment. Therefore, the higher moments have limited practical meaning. The variance together with the mean, however, is an extremely important characteristic of the energy loss distributions. In the local energy density spectra it is, indeed, a useful tool to compare the relative importance of all the different factors involved. Rather surprisingly it turns out that the relative variance is the simple sum of the variances introduced by the individual factors<sup>2,11</sup>. From the local energy spectra the concept may even be extended to cover the biological aspects, and this is a direct connection to the theory of the dose effect relations<sup>3</sup>.

Finally, it should be added that outside the range of our assumption of constant stopping power, the moments are, indeed, a practical means to derive the explicit energy loss distributions. This has been worked out by TSCHALÄR<sup>12</sup>.

## II. Details of the computer program

Formally the method described above looks rather simple. It does not involve anything more than the repeated execution of an integral of the type:

$$g(E) = \int_0^E f(E-x) \cdot f(x) dx \quad (9)$$

Due to the type of functions involved, however, these integrals present considerable numerical difficulties, and it has been a main object in the development of the computer program to find the optimal way to overcome these difficulties.

To illustrate the problems involved we may consider the usual  $1/E^2$  collision law. Take the example of a 5 MeV proton. In this case the maximum delta-ray energy is near to 10 KeV, and  $e_{\min}$  is roughly 0,4 eV. The collision spectrum  $c(E) \sim 1/E^2$  varies very rapidly in the low energy range, so that for the numerical integration one has to work on a point grid with intervals much smaller than one eV. On a fixed linear energy scale that would imply  $10^5$  points for the representation of the distribution. Thus the straight forward approach on a linear grid of equidistant points is out of question; one convolution operation would involve some  $10^{10}$  products.

Therefore, one has to subsegment the integrals or else switch to a new non-linear coordinate system. The latter is the more elegant and more efficient way. One may choose a square root scale or a logarithmic scale in E. Both coordinate systems have their advantages; in the present approach we will choose the simplest and most easy to use method and adopt the more common logarithmic scale.

If on the logarithmic scale one chooses a series of equidistant points to represent the function  $f(E)$ , it turns out that less than 100 points are in general quite sufficient for an accurate approximation. This means that less than  $10^4$  products are involved in the convolution of two distributions; thus the computing times are kept very short. In accordance with the coordinate transformation, however, one has to rewrite equation (9).

Let us assume the following abbreviations:

$$\eta = \ln E, \quad \xi = \ln x, \quad \gamma(\eta) = g(e^\eta), \quad \phi(\eta) = f(e^\eta).$$

Then, as can easily be shown, the integral equation is transformed into:

$$\gamma(\eta) = 2 \cdot \int_{\xi_{\min}}^{\eta - \ln 2} \phi(\ln(e^\eta - e^\xi)) \cdot \phi(\xi) e^\xi d\xi \quad (10)$$

This is still not the most efficient way of performing the integration, since one of the arguments contains exponential functions and a logarithm. This argument may be further simplified:

$$\ln(e^\eta - e^\xi) = \ln(e^\eta(1 - e^{\xi - \eta})) = \eta + \ln(1 - e^{\xi - \eta}) \quad (11)$$

With the additional abbreviation:

$$d(\kappa) = -\ln(1-e^{\kappa})$$

the integral can be written in the following final form:

$$\gamma(\eta) = 2 \cdot \int_{\xi_{\min}}^{\eta - \ln 2} \phi(\eta - d(\eta - \xi)) \cdot \phi(\xi) \cdot e^{\xi} d\xi \quad (12)$$

The functions  $d(\eta - \xi)$  and  $e^{\xi}$  are calculated in advance and need not be computed everytime they are needed. Thus, the integral is again reduced to simple multiplication and addition. The execution is, therefore, fast, and there are no limitations as to the range of energy losses to be covered.

A final remark relates to the zero component in the distributions. While the equations contain these zero components in form of delta function contributions, the zero component and its contribution is, in fact, handled separately in the numerical procedure.

The program is presently available in FORTRAN IV and in ALGOL. Its application is simple, since as input nothing more is required than the read-in of the unnormalized values of the collision spectrum on a logarithmic point grid. One may also state the number of coordinate points on a given interval. Normally 8 points on a factor of 2 are taken, but if highest accuracy is required, one may state the number of 16 or even 32. If one also states a final mean energy loss, one obtains a series of distributions which leads up to the distribution with the desired mean energy loss. The distributions are successively spaced by a factor of two as can be seen from equations (4).

The accuracy of the computations is limited only by the fact that the continuous integrals are substituted by discrete sums. We do not need a detailed discussion of the errors involved,



since the theoretical determination of the moments and the comparison with their numerically obtained values warrant a steady control of the accuracy. With a point grid of 8 points on a factor of 2, and for the usual collision laws the inaccuracy of the mean, the standard deviation, and the second and third central moments is still below 1% after 20 convolutions, a precision good enough for almost all practical applications. Should in special cases highest accuracy be desired, then one may take a finer point grid. Also the linear interpolation in the integration may be replaced by a more accurate one. Presently, however, this appears to be quite pointless.

### III. Practical implications

It is not in the scope of this paper to discuss numerical results of the energy loss calculations. An example may, however, serve to illustrate the new method. In order to give a comparison with the VAVILOV theory, a case will be taken which is not quite out of the range of applicability of this theory. It has to be kept in mind that the differences become much more expressed with smaller mean energy loss.

A 1,58 MeV proton in traversing a tissue equivalent layer of 0,1 micron loses 1,9 KeV on the average. But there are marked deviations from this mean value, as can be seen from recent experiments performed by GLASS and SAMSKY<sup>13</sup>. The VAVILOV theory is in general agreement with the data (see Fig.1). The experimental curve is, however, broader at low and medium energies. This is at least partly due to the electron binding. Unfortunately, we have little information on the actual shape of the collision spectrum at low and medium energies. We do,

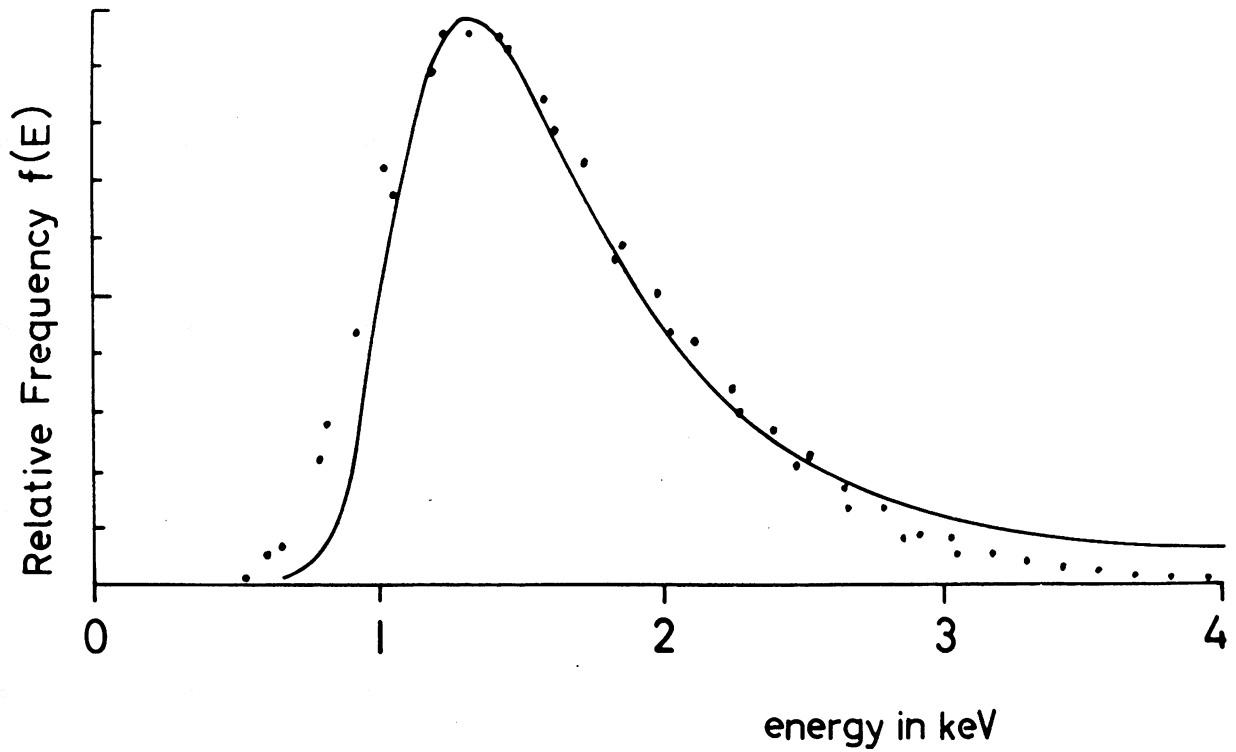


Fig. 1 Probability distribution for the energy deposition of a 1,58 MeV proton in a layer of  $10^{-5}$  gm/cm<sup>2</sup> compared with the VAVILOV theory (according to GLASS and SAMSKY<sup>13</sup>).

however, know that the  $1/E^2$  relation is extremely unrealistic in this range, and the most reasonable guess may at the moment be based on the experimental findings of RAUTH and SIMPSON<sup>14</sup>. It is the shortcoming of these data that they do not extend to energies of much more than 100 eV. Thus one has to interpolate. The interpolation is to a certain degree determined by the condition that the cross-sections above 300 eV as well as the total stopping power have to be kept. Without going into the details we present a modified spectrum in Fig. 2 a. Some of the resulting energy loss distributions in comparison with the ones for the  $1/E^2$  relation are given in Fig. 2 b. The distribution for a mean energy loss of 1,9 KeV is compared with the experimental data in Fig. 3. At low and medium energies this curve is in agreement with the results. Another considerable difference between experiment and theory remains. The experimental values fall off much more steeply at higher energies than the VAVILOV theory predicts. This is clearly due to the loss of delta rays. A treatment which calculates escape and influx probabilities for the different delta rays in a foil of 0,1 micron leads to a good fit at high energies, but the influx of deltas increases the probabilities in the medium energy range much more than is experimentally observed. Therefore, the geometry of a foil seems not appropriate for the experiment, and, accordingly, the probabilities have been calculated for a cylinder of 0,05 micron radius and 0,1 micron length. In this case the energy loss is mostly radial, and there is little influx of delta rays. The resulting collision spectrum is also indicated in Fig. 2 a. This collision spectrum leads to a good agreement with the experimental data over the whole range of energies (see Fig. 4). These remarks should be taken as an illustration, not as a definitive proof for a particular collision spectrum. There are quite a number of interesting questions involved in the problem, and it has to be dealt with in detail.

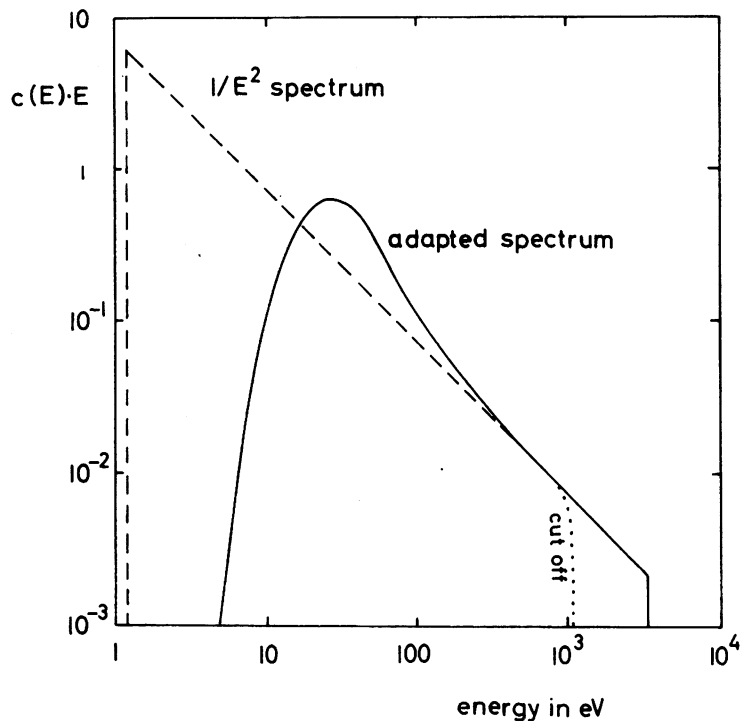


Fig. 2 a The  $1/E^2$  collision spectrum for 1,58 MeV protons, and the modified collision spectra.

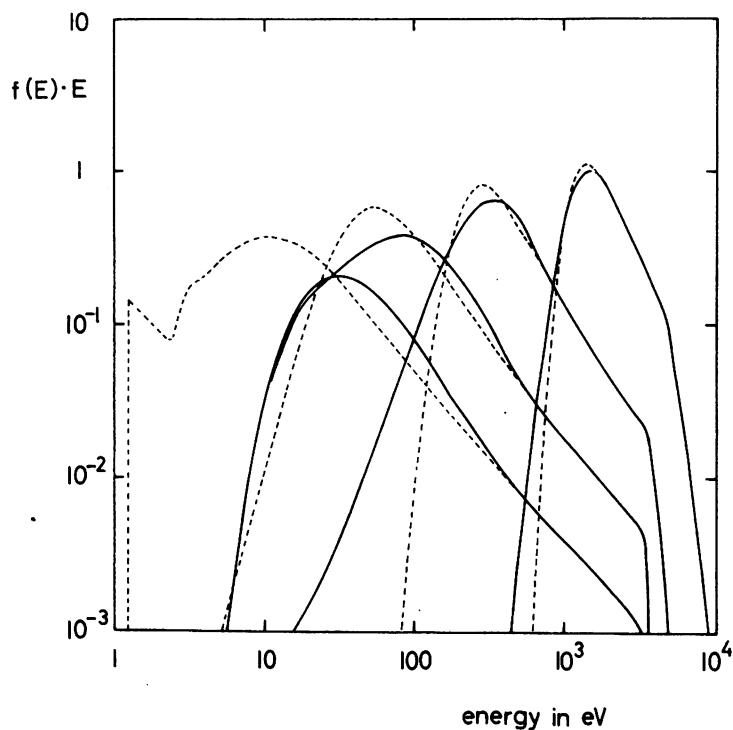


Fig. 2 b Some energy loss distributions for a 1,58 MeV proton according to the  $1/E^2$  collision spectrum (dotted lines) and the adjusted spectrum (full lines). The mean energy loss is: 30 eV, 119 eV, 475 eV, and 1,9 KeV.

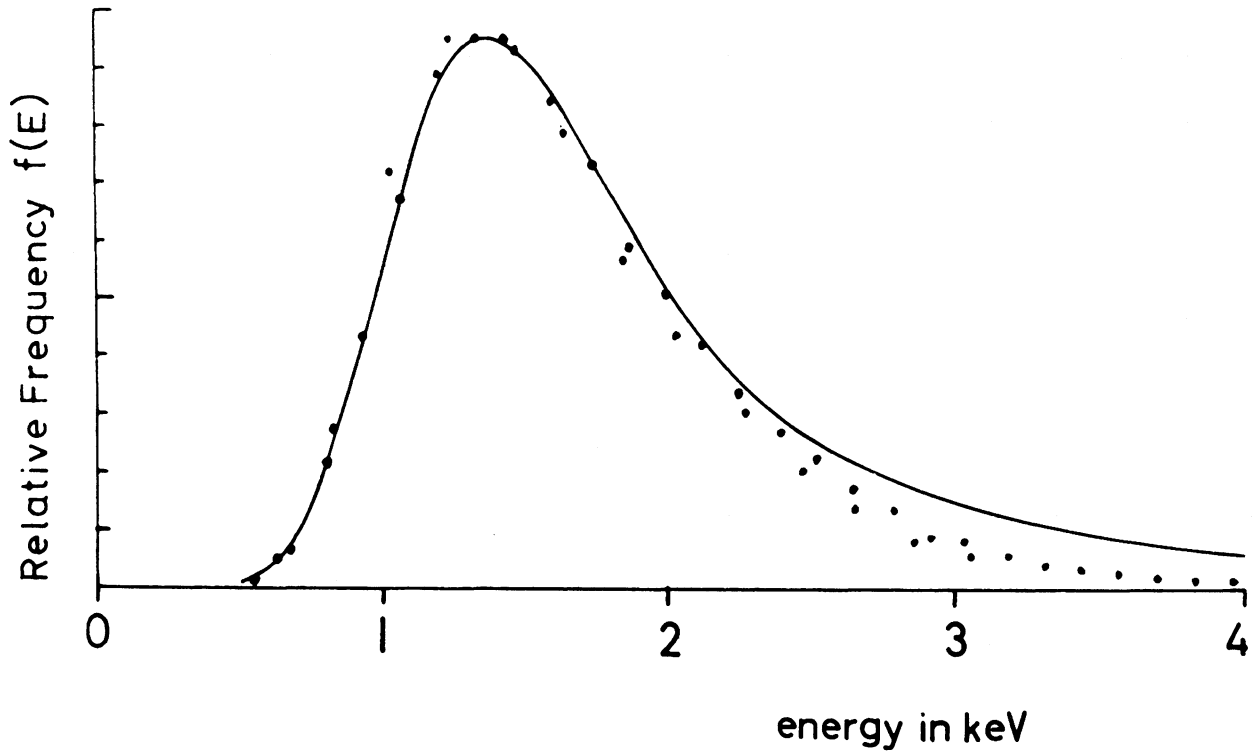


Fig. 3 The experimental data compared with the distribution adjusted at low energies but not corrected for delta-ray escape.

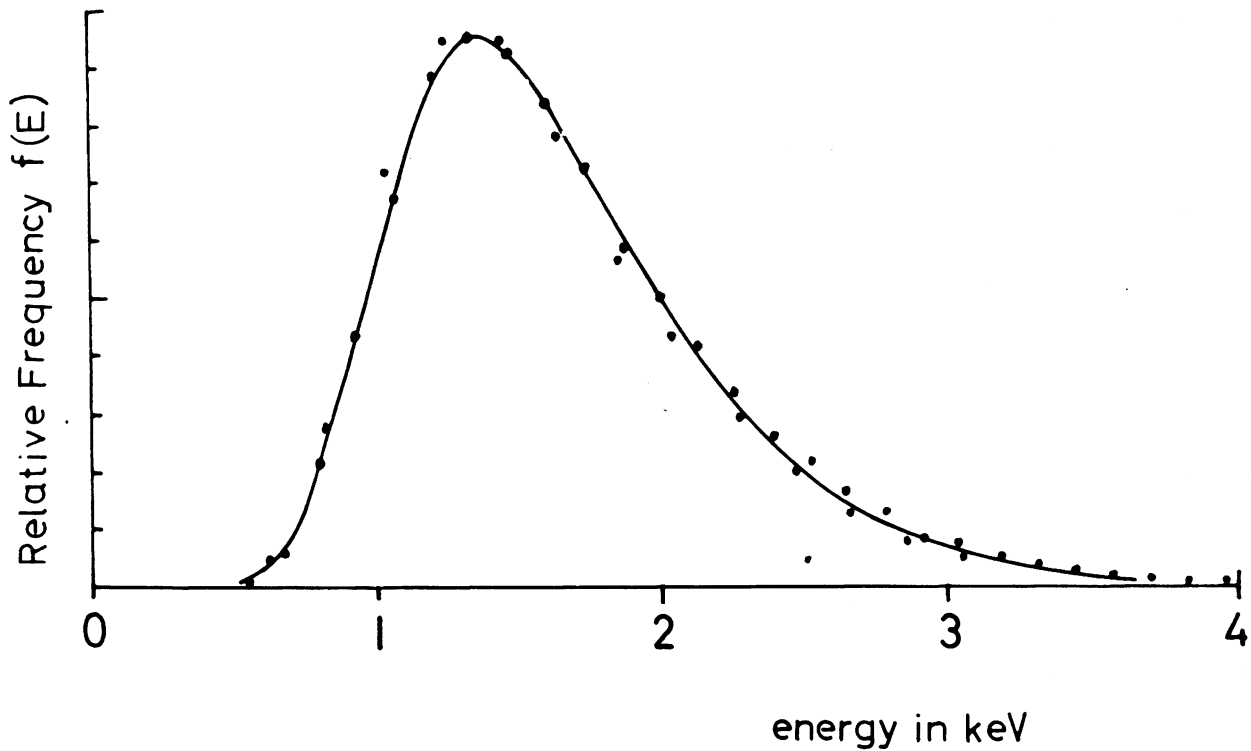


Fig. 4 The experimental data compared with the distribution adjusted at low energies and also corrected for delta-ray escape.

The necessity for a detailed treatment is also the reason that no attempt is made to discuss the derivation of the local energy density spectra with all the factors involved. It may suffice to say that the computer program discussed here is the central building block of an extended version which takes arbitrary collision spectra, LET-spectra, and track length distributions, and puts them together for the actual local energy density distributions,  $P(\Delta Z)$ . The main formulas which govern the inclusion of the LET- and track length-spectra are simple and have been discussed earlier<sup>3</sup> (see also<sup>11</sup>).

The results have to be evaluated in close connection with the experimental data. The experiment is limited at low energies, while the theory, due to the complicated problem of delta-ray escape, runs into difficulties at high energies. This will probably make the best spectra a combination of a theoretical low energy part and a high energy part determined in experiments with wall-less proportional counters.

There is a last point which, in fact, has been the starting point for this work. This is the problem of computing the dose-dependent local energy density spectra  $P(Z)$  from the increment spectra  $P(\Delta Z)$ . It is interesting to note that  $P(Z)$  is in exactly the same relation to  $P(\Delta Z)$  as  $f(E,s)$  is to  $c(E)$ . The reason is that both  $P(Z)$  and  $f(E,s)$  are the result of a Compound Poisson process. That is, they are the result of statistically independent increments. The distribution of increments, i. e. the spectrum of the Poisson process, is  $P(\Delta Z)$  in the one case, and  $c(E)$  in the other. Thus the computer program which is a general solution of the Compound Poisson process can be used for both problems without any change. The only difference is in the shape of the spectra. The distributions  $P(\Delta Z)$  are easier to handle than some of the extremely skew collision spectra  $c(E)$ .

Indeed, the derivation of the  $P(Z)$  spectra from the single event spectra  $P(\Delta Z)$  has been done first. It was B. BIAVATI who has developed a rigorous program for this purpose<sup>15</sup> which in contrast to the Monte Carlo calculations<sup>3</sup> produces exact solutions. His method lies in a similar direction as the present approach. As a matter of fact the work reported here has been greatly stimulated and advanced by the close cooperation with the working group at the Columbia University Radiation Research Laboratories.

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