ICANS-VI
INTERNATIONAL COLLABORATION ON ADVANCED NEUTRON SOURCES
June 27 - July 2, 1982

COMPUTATIONAL METHODS FOR HIGH-ENERGY SOURCE SHIELDING

T.W. Armstrong*, P. Cloth, D. Filges

Institut für Reaktorentwicklung
Kernforschungsanlage Jülich GmbH
Postfach 1913
D-5170 Jülich 1, Germany

*KFA Consultant, P.O. Box 2807
La Jolla, California 92038, USA

ABSTRACT

The computational methods for high-energy radiation transport related to shielding of the SNQ-spallation source are outlined. The basic approach is to couple radiation-transport computer codes which use Monte Carlo methods and discrete ordinates methods. A code system is suggested that incorporates state-of-the-art radiation-transport techniques. The stepwise verification of that system is briefly summarized. The complexity of the resulting code system suggests a more straight forward code specially tailored for thick shield calculations. A short guide line to future development of such a Monte Carlo code is given.

COMPUTATIONAL METHODS FOR HIGH-ENERGY SOURCE SHIELDING

T.W. Armstrong*, P. Cloth, D. Filges

Institut für Reaktorentwicklung
Kernforschungsanlage Jülich GmbH
Postfach 1913
D-5170 Jülich 1, Germany

*KFA Consultant, P.O. Box 2807
La Jolla, California 92038, USA

INTRODUCTION

The SNQ shielding problem has special features and importance compared to usual accelerator shielding considerations. It presents difficult computational requirements because of the combination of a relatively high-energy source, large shielding dimensions, and geometric complexities. There does not presently exist a computer code system with an appropriate data base which is directly applicable to the SNQ shielding problems of concern.

In the following discussion, the step-wise development of such a shielding code system is suggested. The basic approach is to couple radiation computer codes which use both Monte Carlo methods (suitable for complex geometries) and discrete ordinates methods (suitable for deep-penetration) with a cross section data base extended to accomodate the SNQ beam energy of 1100 MeV. Further plannings to improve the system aiming at an all-Monte-Carlo procedure capable of deep penetration problems are outlined.

The main factors governing the bulk shield thickness required are the attenuation of high-energy particles (mainly neutrons) and the material density. This is because the flux (or dose) attenuation depends approximately exponentially on these factors, and only linearly with source strength (and dose rate criterion). That is, the flux spectrum at large distances (several mean free paths) from the source is roughly represented by

$$\Phi(E,x) \propto S \cdot f(E) \cdot \exp(-x\rho/\lambda_{att})/x^2. \qquad (1)$$

This can be seen e.g. in Fig. 1 from measurements and calculations. For the depht-dependence of high-energy particles see also Refs. 1 and 2.

In detailed code calculations the quasi material constant λ_{att} is not valid. In lieu of it the corresponding differencial cross section data are used. Providing of cross-sections will be discussed.

One might expect that since λ_{att} is so fundamental to shield design for high-energy radiations, accurate values for common shielding materials would be available from previous experiments and accelerator facility designs. This is not the case. For example, previous measurements of attenuation lengths for iron range from about 120 to 180 g/cm^2. (An HETC code calculation for a 500 MeV proton source and iron shield is reported by Broome to give λ_{att} = 179 g/cm^2 /3/.) There is also a wide range of measured λ_{att} values reported for concrete ($\approx$110 to $\approx$ 172 g/cm^2). (A summary of all but the most recent measured values for λ_{att}, and descriptions of most of the experiments, is given in /4/.)

There are several reasons for these large variations in the measured values for λ_{att}. Some unaccounted for invalid assumptions have to be made in the measurements. Also λ_{att} has some spectral dependence, e.g., λ_{att} measured along the beam axis can be different from off-axis measurements because of differences in particle spectra.

SUGGESTED METHOD FOR SHIELDING CALCULATIONS

There are, of course, some alternatives as to the most appropriate calculational approach to take. However, only one procedure is outlined here, which is believed to be feasible and reasonably accurate, but which can probably be improved with further thought.

The basic approach here for the near future is to use a combination of Monte Carlo and discrete ordinates methods. While in principle it is feasible, even for the very thick shields envisioned, to use Monte Carlo methods alone, this would require some substantial modifications of existing codes, or eventually writing of new codes. This will be discussed later as an further improvement. The method outlined here can be applied nearer term.

The main advantage of the code system is that it incorporates state-of-the-art radiation transport developments and is, we believe, representative of the most accurate methods allowed by present day cross section data and computer capabilities.

The radiation transport codes suggested for use in the shielding code system are: 1. HETC /5/, for the Monte Carlo calculation of high-energy nucleons and pions, 2. MORSE /6/, for the

Monte Carlo transport of low-energy and γ-rays, 3. the discrete ordinates code ANISN /7/, for one-dimensional neutron and γ-ray transport, and 4. the discrete ordinates code DOT /8/, for two-dimensional neutron and γ-ray transport. It should be noted that, except for HETC, other comparable transport codes exist. In particular, there is the Los Alamos group of transport codes: the MCNP (continuous energy) and MCMG (multigroup) Monte Carlo codes /9/, which have capabilities similar to MORSE; and the discrete ordinates codes for 2-D and 1-D transport, TWOTRAN and ONETRAN /10/. The reasons for selecting MORSE, ANISN and DOT for the shielding code system are, in addition to representing state-of-the-art capabilities, they are compatible with the present IBM computer facilities at KFA and with the needed high-energy cross section data base.

COMPUTER CODES

Monte Carlo Codes

The high-energy transport code HETC and the low energy neutron/γ-ray transport code MORSE, which have been applied extensively during the SNQ reference design study /11/, would be used in the shielding calculations in their present form. It would however, probably be better to couple these two codes at a higher neutron energy (say 60 MeV) than that usually used (15 MeV). This could be done by extending the MORSE cross section to higher energies using the HILO library discussed below. This change is expected to have a negligible effect on bulk shielding estimates. However, it may be important in obtaining the high-energy portion of the neutron spectrum from the SNQ-neutron moderator. High-energy neutrons in the moderator which elastically scatter with oxygen would be more accurately treated by making this change.

Discrete Ordinates Codes

The discrete ordinates, or S_n, method is a means of numerically solving the Boltzmann transport equation in which the phase space is divided into a number of discrete points. A set of finite differences equations can then be formulated which can be solved by an iterative technique. (The detailed equations are given, for example, in Ref. /12/).

The radiation transport codes ANISN and DOT employ the discrete ordinates methods coupled with a multigroup deterministic solutions of the Boltzmann transport equation for neutrons and gamma rays. ANISN solves the one-dimensional form of the Boltzmann transport equation in slab, cylindrical or spherical geometries, whereas DOT solves the two-dimensional form in slab and R-Z or R-θ cylindrical geometries.

While ANISN is only 1-D, the computation and set-up times are much less than for DOT. Thus, ANISN will be very helpful in evaluating cross section sets, doing sensitivity studies, investigating parameter variations, etc. which would be too time consuming if only DOT were used.

Code Coupling Considerations

The ANISN and DOT codes transport only neutrons and (for appropriate cross section input) the secondary gamma-ray produced by neutrons. Therefore, a basic premise of the Monte Carlo/discrete ordinates coupling procedure suggested here is that the discrete ordinates codes are used only for transport in those spatial regions of the shield where neutrons are the dominate particles. One method of coupling is to consider an internal boundary in the shield at some depth sufficiently large that neutrons dominate. The Monte Carlo calculated neutron current across this boundary then constitutes the discrete ordinates code input. Both ANISN and DOT allow a boundary angular neutron source as an input option, so no code modifications are required.

"Coupling codes" will have to be written to put the Monte Carlo results in the quadrature set format needed to provide the neutron source for ANISN and DOT. HETC has previously been coupled with ANISN /13/, but for a volumetric ANISN neutron source and not for deep-penetration applications. A code called DOMINO /14/ for the opposite type of coupling, i.e., DOT output to Monte Carlo, is available. However, we are not aware of any previously documented experience in coupling Monte Carlo transport followed by discrete ordinates transport for the very deep penetration shielding applications of interest here.

All neutrons from the Monte Carlo calculations crossing the coupling plane in the "positive" (larger depth) directions for the first time then constitute a surface source for the ANISN or DOT calculations. This is illustrated in Fig. 2.

The coupling plane for defining the source for the discrete ordinates calculations should be located sufficiently deep into the shield that the neutrons are the dominate high-energy particles rather than protons, but yet no deeper than necessary to satisfy this criterion so that the statistics from the Monte Carlo calculations are as good as possible. Fig. 3 gives a good picture of the neutrons becoming the dominate high-energy cascade particle. It is also advantageous to have the coupling plane as shallow as possible so that there will be a "region of overlap" where results from the two calculations can be compared.

DATA BASES

The shielding code system suggested requires high-energy multigroup cross section data for the discrete ordinates transport calculations. Much of the needed cross section data are available, but the present data base is not completely compatible with SNQ application requirements because the maximum neutron energy considered is 400 MeV. Also, there are other approximations in the present data base whose accuracy is questionable for the very thick shields of interest for the SNQ.

The approach suggested here is to make ad hoc modifications to the present data to allow "Phase I" calculations to be made, which would include transport calculations to test the importance of present approximations.

Status of Present High-Energy Transport Cross Section Data Base

A multi-energy group cross section library (called HILO) for coupled neutron/γ-ray transport has recently been developed at ORNL in a format compatible with ANISN and DOT input requirements /15/. Features of this library are summarized in Table II. These data have been obtained by using experimental data at low energies (< 14.9 MeV) and theoretical models at high energies (14.9-400 MeV).

Some work has also been done at Los Alamos /16/ to obtain two high-energy cross section sets: 1. a 60 group library from thermal to 60 MeV, and 2. a 41 group library up to 800 MeV. The 41 group library contains the following elements: H, C, O, Al, Si, Fe, Mo, W, and Pb. A P_3 angular expansion is used for all elements except Fe, which is extended to P_8. These cross sections were obtained in a manner similar to that of the HILO library, i.e., ENDF data at low energies (<=20 MeV) and optical model and intranuclear-cascade-evaporation model calculations for higher energies.

It should be noted that the Los Alamos cross section library does not include elastic scattering for nuclides other than H at high energies. Based on a test case for an iron shield (a rather "thin" one-dimensional spherical shield having diameter of 1.4 meters with a central isotropic neutron source from 50 MeV deuterons on Be), it was concluded that high-energy elastic scattering had a negligible effect on the dose equivalent at the edge of the shield /16/. However, calculations for a heavy concrete shield reported in Ref. /17/ (using the HILO library, for a spherical shell shield 3.7 m thick, point isotropic neutron source, <~60 MeV, from deuterons Li) show that the dose equivalent outside the shield is over estimated by more than three orders of magnitude if elastic scattering by heavy (other than H) elements at high energies (>=14.9 MeV) is neglected. (This may also have implications for the SNQ bulk shielding calculations in comparing iron vs. cast-iron since cast-iron contains nominally 20 atom per cent C and Si).

It is suggested here that the HILO high-energie cross section library be used (with modifications to allow higher-energies) for the initial discrete ordinates calculations related to SNQ shielding. The main consideration is that this data set includes elastic scattering (for all but the heaviest nuclei - W and Pb) whereas the Los Alamos library does not. Also, the HILO library includes γ-ray production and transport cross sections for γ-rays produced in low-energy (< 14.9 MeV) neutron collisions, which are neglected in the Los Alamos library. Furthermore, the HILO library has a higher order angular expansion at high energies (p_5 vs P_3), except for Fe, and a finer energy group structure.

While the HILO library is recommended, it should be noted, however, that some of the considerations and assessments mentioned in Ref. /16/ in connection with the development of the Los Alamos library are very relevant to our interests. As an example, for the high-energy nonelastic cross sections of the HILO library, the results of intranuclear-cascade-evaporation model calculations are used directly above $\approx$60 MeV. In the Los Alamos library, such model cross sections are adjusted in some cases (e.g., upward by about 15 % for Fe) where some experimental data points are available.

SNQ-SHIELDING CALCULATIONS

Several "baseline" configurations are suggested here for setting up the initial shielding code system. There are a number of questions to be investigated using these simple shield arrangements, as outlined and discussed below.

Both 1-D and 2-D arrangements are suggested. The reasons for starting with a 1-D setup are: (a) To gain experience in Monte Carlo/discrete ordinates coupling with the simpler 1-D case. (There are no data presently available to check either the 1-D or 2-D cases, but the laterally integrated 2-D results can be compared with the 1-D calculations as a partial check.) (b) The 2-D calculations will require considerable computer time for deep penetrations, and many of the preliminary calculations (investigating quadrature sets, parameter variations, etc.) can be made with the 1-D set-ups. (c) For some of the eventual applications (e.g., accelerator shielding requirements due to proton beam losses) 1-D approximations are adequate.

Baseline Arrangements

A source/shield arrangement in cylindrical geometry for the 1-D case is shown in Figure 4. This set-up serves for baseline test calculations. Fig. 5 shows (upper case) a similar set-up for DOT calculations.

The lower arrangement in fig. 5 is to allow early estimates of bulk shielding dimensions using the initial code system and data base. The couplig surface is the target surface in this case.

Note also that the 1-D arrangement preserves the anisotropy of the neutron source at the coupling plane, so, for example, investigations of appropriate quadrature sets from the 1-D ANISN calculations should be relevant to the 2-D DOT calculations.

A target diameter of 10 cm is chosen to be consistent with the thickness of the reference design target wheel. We have indicated a target length L as approximately the range R of the primary proton range so that primary protons have a chance to produce neutrons within the target material. The angular and radial dependence of the neutrons at the coupling plane will depend upon L (the magnitude depending on L and the depth of the coupling plane). For example, for the reference design target wheel, where the wheel diameter was >~2 range thicknesses, relatively few neutrons escape the target in the forward (0°) direction, and the neutron angular distribution is peaked at about 30°. Therefore, calculations for several target lengths (e.g., $L=0$, L R, and L 2R) would be of interest.

Arrangement with Beam Holes

Prediction of the doubly differential neutron and gamma-ray spectra emerging from a beam hole, taking into account interaction effects in the shield material around the hole, is a very demanding calculation. It will require the full extent of the transport codes as well as computer capabilities.

The first part would be to calculate the angular and spatially dependent neutron, proton, and charged pion energy spectrum leakage from the target surfaces adjacent to the moderators. The moderators should be included in these calculations to account for any second order effects; that is, particles which are "reflected" from the moderator back into the target region may produce additional particles which then can enter the moderator. A MORSE calculation will also be required to account for the neutrons which are produced in HETC below the cutoff energy. These spectra obtained become the source for part two of the HETC-MORSE calculation.

The second part of the calculation need only include the moderator since all back-scattered particles have been accounted for. The source calculation for the second HETC calculation will be the protons, charged pions and neutron leakage spectra obtained in the first part of the calculation. MORSE will be used twice during this step of the calculation: once to transport the low-energy neutrons leaking from the target, and once to transport the neutrons produced in the second HETC calculation. By using some of the biasing techniques already incorporated into the MORSE code, an improvement in the statistical accuracy of the low energy emerging neutrons can be obtained. It may also be necessary to incorporate some biasing techniques into HETC - for example, particle splitting in important regions and directions.

The DOT calculation will probably require a biased (asymmetric) angular quadrature, with most of the angles pointing down the collimator hole. In addiation, it will be necessary to define fine radial intervals (say ~ 0.1 cm) for a short distance (~ 1 - 2 cm) into the shield material to properly account for "skin" effects. Since neutrons and gamma rays which are located more than several mean-free-paths into the shield material have little effect on the emerging particles at the end of the collimator, it is only necessary to make the thickness shield material surrounding the beam hole a few mean-free-paths thick. There is not, of course, experience to guide any of the above assumptions and test calculations will be necessary to refine the procedure. The arrangement is shown in Fig. 6.

It is not clear whether a single DOT calculation can simulate the entire length of the collimator. This is because the length-to-diameter ratio is very large (L/D ~ 60) and a fine spatial grid is needed radially near the collimator surface. Therefore, array sizes may exceed computer storage capacities, and/or computation times may be prohibitive. If this should be the case, the problem can be divided into several parts, "overlapping" several DOT calculations for sequential segments of the collimator length (see Fig. 6). (This procedure is suggested by "overlap" discrete ordinates calculations which have been made for deep penetrations in air from neutron sources /18/.

FUTURE CODE SYSTEMS AND DATA BASE

The complexity of the presented code system ,the computer time and man power consuming running procedure for each problem case suggest a more straight forward computer code specially tailored for thick shielding calculation. If we realize the constraints of the above system, e.g., the strongly limited geometric capabilities, or the restriction to only neutral particle treatment (usually neutrons and gammas), we find, that Monte-Carlo techniques is the adequate means that should be tried for our purpose.

Thick Shield Monte Carlo Codes

The following is somewhat qualitative and serves only as a guide line in developing a special thick-shield Monte Carlo code. In thick shields as they occur in the SNQ case párticles have to travel a large number of mean free paths to go through, whereas the average number of collisions that particles undergo during their lifetime (until energy has fallen below a certain level) is considerably smaller. Neutral particles, however, can travel any distance between collisions with, of course, low probability for larger path-lengths. Thus, a few particles can penetrate the thick shield, and the calculation of this small fraction is the deep penetration problem.

For simplicity reasons let us asume that the shield consists of only one single material and forget about the fact that the considered particle may change its identity from collision to collision and temporily may be a charged particle. This will only complicate the computational procedure but not affect the principle. The collision points of the particle tracks will be, according to what was discussed above, concentrated close to the source, with more or less none of them in the far away shield regions near the surface. What is needed, however, is for bulk shielding calculations collision points near the surface, and for the case with beam tubes a more flat distribution.

The idea now is to calculate first a collision history of a particle without considering beforehand the free paths between collisions. This is justified as in our simpel model collision physics is space independent. After that, we sample a set of free tracks that has importance for our purpose. We do this in a way that the total migration length, that is the sum of all free paths of a track is in a certain range of high importance. Although there is some similarity to so called path-length stretching, which produces a wide variety of migration lengths, our procedure - and this is the advantage - gives control over the important parts of this variety.

Let us express the migration length in terms of the mean free path and denote it η, then the conditional probability of a collision history for agiven relative migration length η is a measure for the importance of this history to penetration of a shield of the thickness in the order of η. According to our discussion above η the number of mean free paths through the shield is (on average) larger than n the number of collisions.

While the bulk of histories has n values (collision numbers) near the average and well below η, there might be a small fraction of histories with n close to η having thus an extremely high importance yet being completely underrepresented in the n distribution provided e.g. by the intra-nuclear cascade calculation, as compared to their relevance for the shielding calculation (Fig. 7). It is not known how strong this effect could be, but it can be overcome by using biasing techniques already in the intra-nuclear cascade model, which is a Monte-Carlo program itself. Obviously it is the extremely forward directed component of the cascade variety of extreme low energy loss, that can have exceptional high collision numbers. If this small history group plays a certain role, for which we have some indication, it has also to be considered in preparing cross-sections with HETC for use with the near term Monte-Carlo discrete ordinate system. So one of our next steps in code development is introduction of suitable biasing techniques in the intranuclear cascade part of HETC.

REFERENCES

1 S.P. Shen

Passage of High-Energy Particles in Matter:
Nuclear Cascades Induced in Dense Media by 1-and 3-GeV Protons
BNL-8721,Brookhaven National Laboratory (1965).

2 T.W. Armstrong and R.G. Alsmiller
Monte Carlo Calculations of the Nucleon-Meson Cascade in Iron Initiated by 1- and 3-GeV Protons and Comparisons with Experiment
Nucl. Sci. Engr. 33, 291 (1972)

3 T.A. Broome
Shielding for the Spallation Neutron Source at the Rutherford Laboratory
Paper in "Meeting on Targets for Neutron Beam Spallation Sources"
G.S. Bauer (Ed.), Jül-conf-34, Januar 1980

4 W. Wade Patterson and Ralph H. Thomas
Accelerator Health Physics
Academic Press, New York, New York, 1973

5 T.W. Armstrong and K.C. Chandler
HETC - A High-Energy Transport Code
Nucl. Sci. Engr. 43 353 (1971)

6 E.A. Straker
The MORSE Code - A Multigroup Neutron and
Gamma-Ray Monte Carlo Transport Code
ORNL-4585, September 1970

7 W.W. Engle, Jr.,
ANISN, A One-Dimensional Discrete Ordinates
Transport Code with Anisotropic Scattering,
K-1693, March 1967
(also updated features described in ANISN
Code Package as distributed by the Radiation
Shielding Information Center, Oak Ridge, TN)

8 W.A. Rhoades, et.al.
The DOT-IV Two-Dimensional, Discrete-Ordinates
Transport Code with Space-Dependent Mesh and
Quadrature
ORNL-TM-6529, August 1978
(also, related documentation contained in DOT-IV
Code Package distributed by the Radiation Shielding
Information Center, Oak Ridge, TN)

9 W.L. Thompson and E.D. Cashwell
The Status of Monte Carlo at Los Alamos
LA-8353-MS, May 1980

10 T.R. Hill
ONETRAN, A Discrete Ordinates Finite Element Code
for the Solution of the One-Dimensional Multigroup
Transport Equation
LA-5990-MS, June 1975

11 T.W. Armstrong, P. Cloth, D. Filges, R.D. Neef
Theoretical Target Physics Studies for the SNQ
Spallation Neutron Source
Jül-Spez-120, July 1981

12 F.R. Mynatt, F.J. Muckenthaler, and P.N. Stevens
Development of Two-Dimensional Discrete Ordinates
Transport Theory for Radiation Shielding
CTC-INF-952, August 1969

13 T.W. Armstrong
Calculation of the Lunar Photon Albedo from
Galatic and Solar Proton Bombardment
J. Geophys. Res. 77, 524 (1972)

14 M.B. Emmett, C.E. Burgart, and T.J. Hoffman
DOMINO, A General Purpose Code for Coupling Discrete
Ordinates and Monte Carlo Radiation Transport Calculations
ORNL-4853, July 1973

15 HILO, 66 Neutron, 21-Gamma-Ray Group Cross Sections for
Radiation Transport for Neutron Energies up to 400 MeV
ORNL Radiation Shielding Information Center Data Package
DLC-87 (1981)

16 W.B. Wilson
Nuclear Data Development and Shield Design for Neutrons Below 60 MeV
LA-7159-T, February 1978

17 R.G. Alsmiller, Jr., and J. Barish
Neutron -Photon Multigroup Cross Sections for Neutron Energies < 60 MeV
Nucl. Sci Engr. 69, 378 (1979)

18 J.V. Pace, III, F.R. Mynatt,and L.S. Abbott,
"A Study of the Overlap Conditions Required in Sequential Discrete Ordinates Transport Calculations for a 14-MeV Neutron Source in a 5000-m Radius Cylinder of Air",
ORNL-TM-3269, June 1971

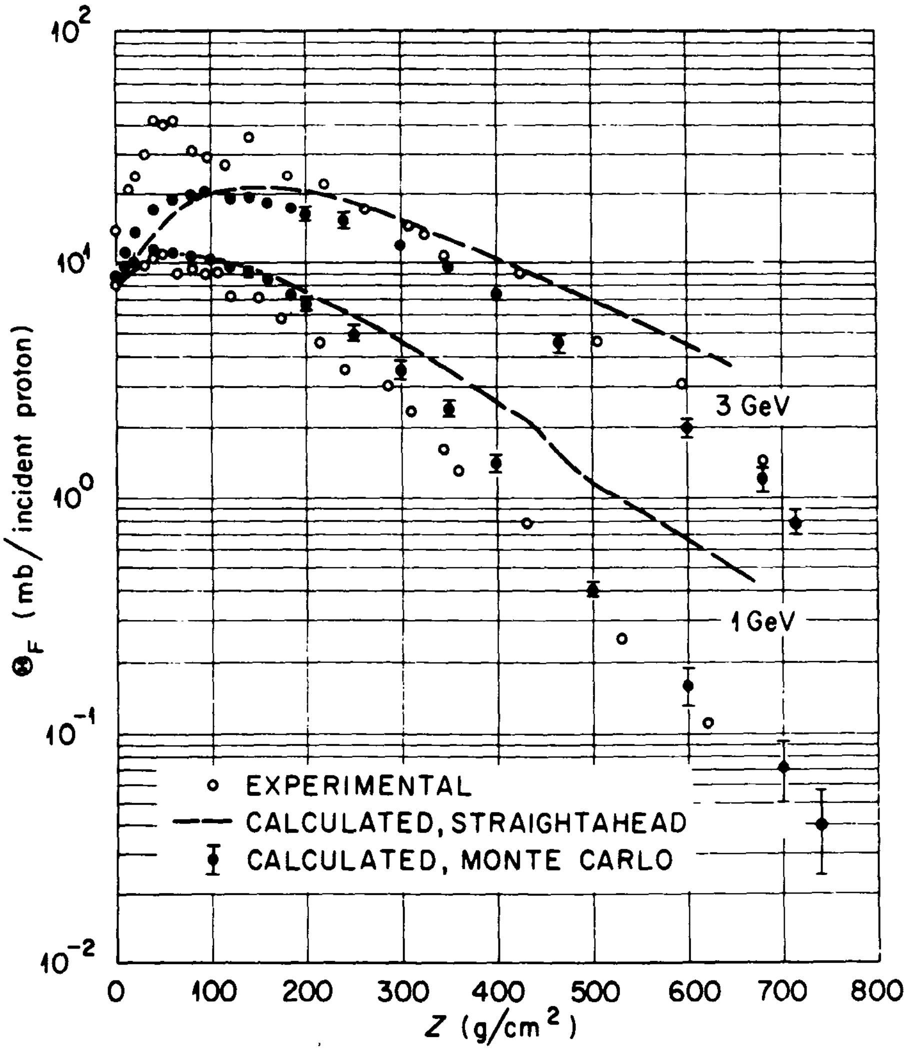

Fig. 1
Depth-dependence of high-energy particles in an iron shield bombarded by 1 and 3 GeV proton beams. (F-18 production in Al foils)
The experimental values are taken from Ref. 1, the calculated values from Ref. 2.

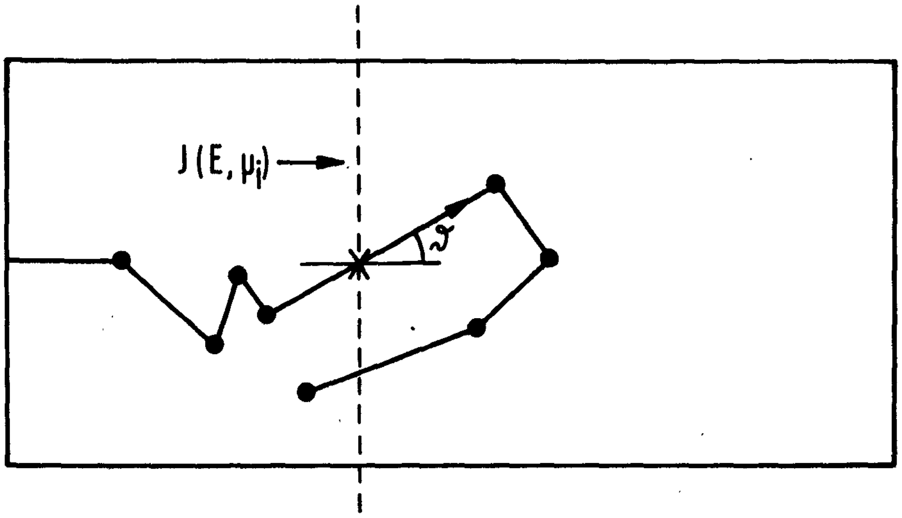

Fig. 2
Schematic of the contribution of a particle to the surface source at its first crossover point on the surface.

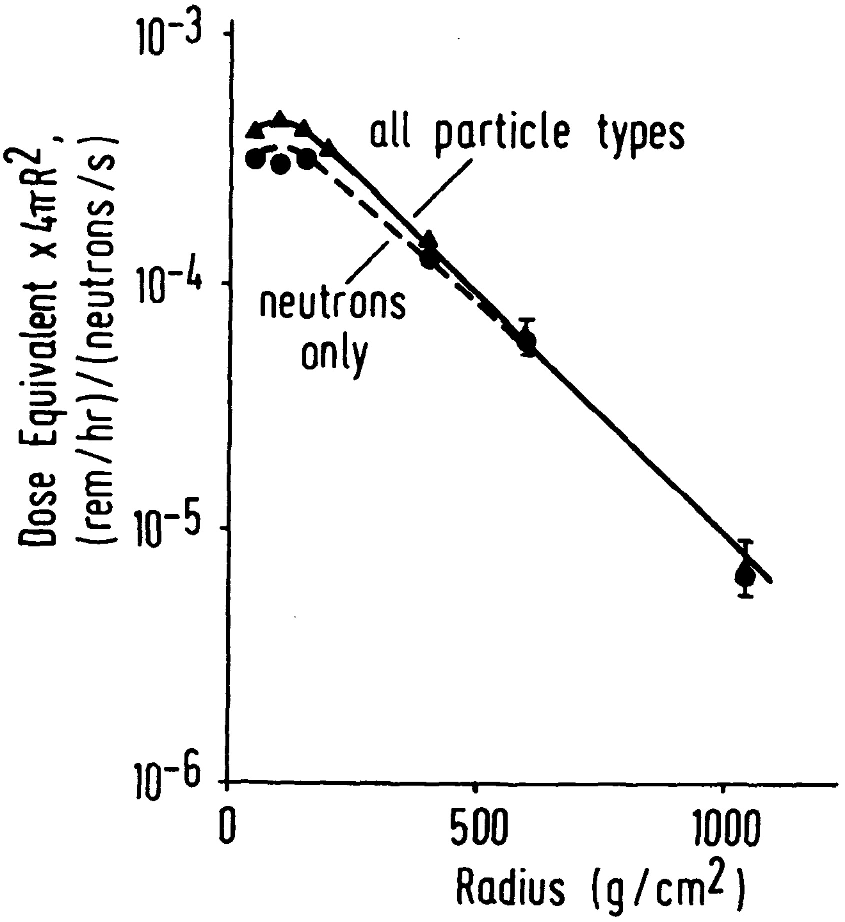

Fig. 3
Example showing that after a few high-energy mean-free-paths in the shield, the dominate particles are neutrons. This example is for the biological dose at the outside of a spherical iron shield due to an isotropic point source of 500 MeV neutrons, as calculated using the HET code.

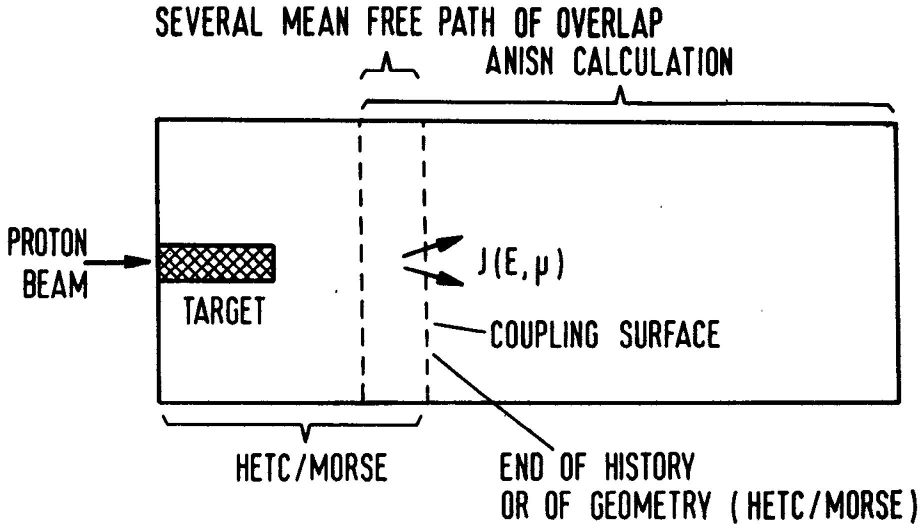

Fig. 4
1-D arrangement for source/shield test calculations in cylindrical geometry.

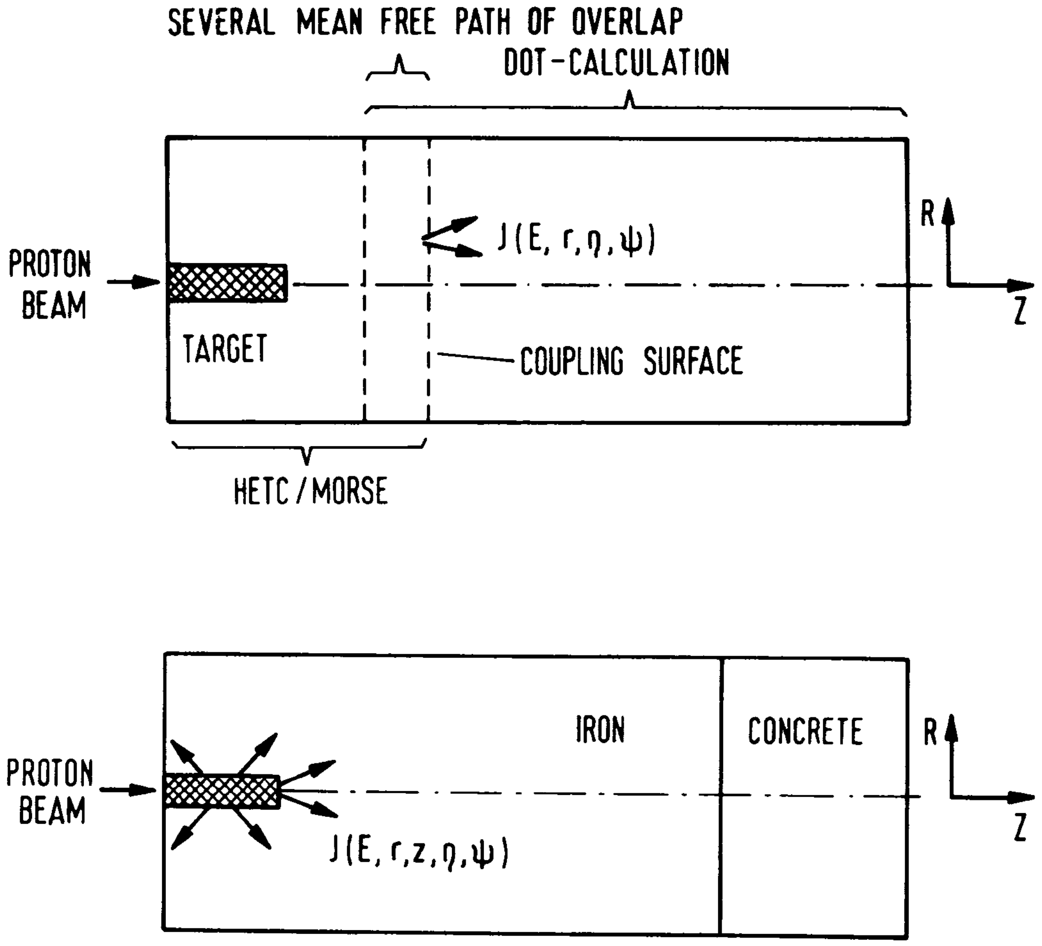

Fig. 5
2-D arrangement for test and early bulk shielding calculations using DOT in cylindrical geometry.

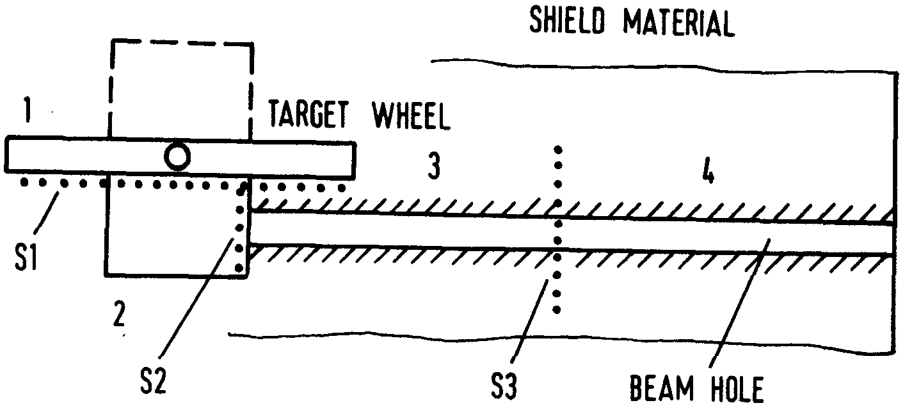

Fig. 6
Arrangement for 2-D SNQ-beam hole calculations with code coupling surfaces S1, S2 and S3.

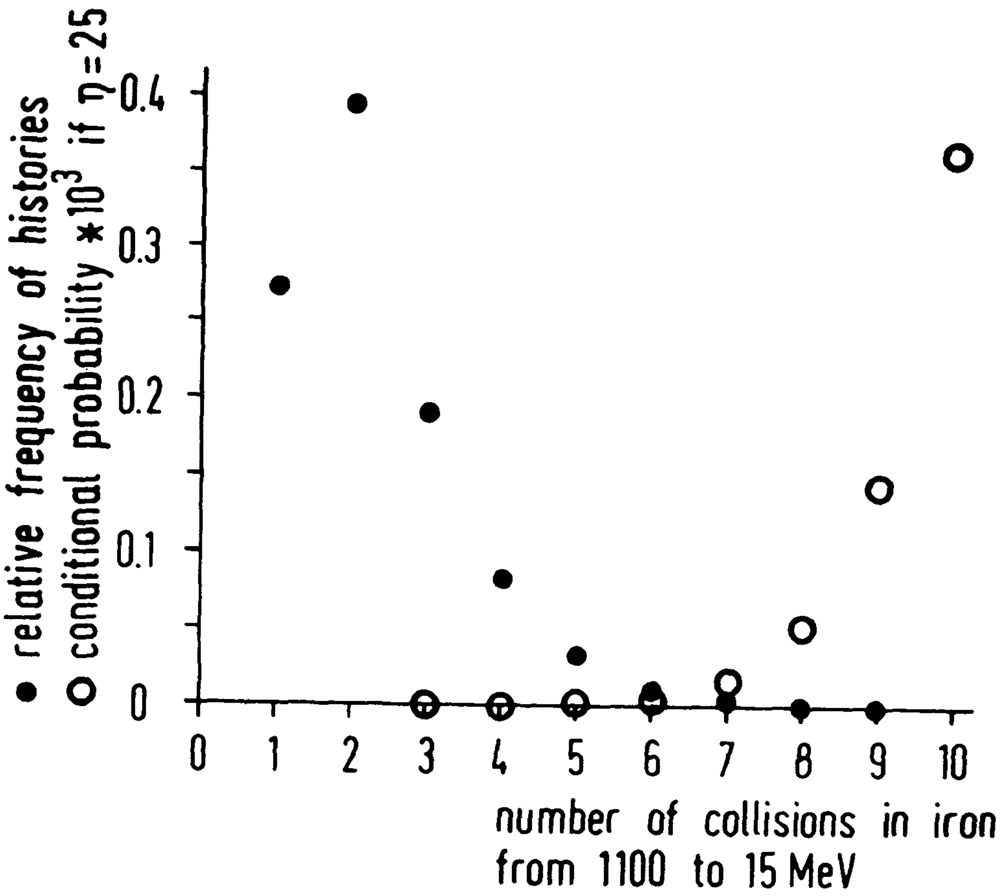

Fig. 7
Relative frequency of a particle collision history compared to its probability in penetrating a thick shield.