APPLICATION OF MONTE CARLO METHOD TO NEUTRON SHIELDING IN ORDINARY CONCRETE

BY

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DECLARATION

It is hereby declared that:

1. The report presented in this thesis is a result of research carried out by the author.
2. This thesis has not been submitted in whatever form to any other institution, organization or body, for the award of any degree.
3. All inclusions from the work of others have been duly acknowledged.

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CERTIFICATION

This thesis entitled - APPLICATION OF MONTE CARLO METHOD TO NEUTRON SHIELDING IN ORDINARY CONCRETE by DANIEL YAKUBU KUTCHIN meets the regulations governing the award of the degree of MASTER OF SCIENCE of Ahmadu Bello University, and is approved for its contribution to knowledge and literary presentation.

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ABSTRACT

Using the Monte Carlo formalism we have calculated the thickness of ordinary concrete required to shield a source of 14 MeV neutrons. A shield thickness of (2.3 ± 0.2) meters was obtained. This is in good agreement with the results given in the MBS (National Bureau of Standards) Handbook 63 (1957) and the ORINS (Oak Ridge Institute of Nuclear Studies) Journal (1963) using the Removal cross section technique. Both quote 2.1 and 2.6 meters respectively.

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Chapter 1

INTRODUCTION

1.1 Purpose of the Project

The purpose of a radiation shield is to protect objects that are vulnerable to radiation damage from being irradiated. The present work seeks to utilise the Monte Carlo formalism to calculate the thickness of an ordinary concrete shield required around the neutron generator due to be installed at the Physics Department of Ahmadu Bello University, Zaria

This work was inspired by the desire to establish a rigorous approach to the shielding of neutrons, particularly, 14 MeV neutrons. So far such work has not been undertaken. In its regulations governing the shielding of fast neutrons within the broad range of up to 30 MeV, the NBS (National Bureau of Standards) handbook 63 (1957) recommends a shield thickness of 2.1 meters for ordinary concrete. The Bureau based its findings on a source of prompt fission neutrons, whose energy spectrum is quite unlike that of the neutron generator. The ORINS (Oak Ridge Institute of Nuclear Studies) gives a shielding requirement of 2.6 meters for ordinary concrete. Both results are obtainable from the approximate relation

$$\phi = \phi_o B e^{-\Sigma_r x}$$

where ϕ_o = initial flux,

B = buildup factor (=5),

Σ_r = removal cross section

= 0.094 (NBS)

= 0.075 (ORINS)

x = Shield thickness, and

ϕ = guidance flux

= 10 neutrons/cm^{2}sec

Cloutier (1963), who actually performed a study of a neutron generator, designed a shielding arrangement accomplished by about 3.7 meters of distance that included shielding consisting of 70 centimeters of water and 40 centimeters of concrete. Beside the fact that an empiricist technique was employed, the work is not specific about the amount of shielding that would be required if only concrete was used as the shield material.

1.2 The Neutron Generator

The neutron generator of this study is a Cockcroft-Walton type of accelerator, model A711, made by Kaman Sciences. The particles normally accelerated are ionised hydrogen or deuterium produced in a radio frequency ion source. A full description of the unit may be found in the instrument manual provided.

When the ion beam hits the target material, nuclear reaction between the target material and the beam occurs, producing neutrons:

$$ {}^{2}_{1}H + {}^{3}_{1}H \rightarrow {}^{4}_{2}He + {}^{1}_{1}n $$

Reaction energy = +17.3 MeV

Neutron energy = 14.3 MeV

The advantages of the model (A711) include:

i. the reduction of x-ray production due to the efficient beam focussing ability of the lens assembly and a pressure condition of 0.015 Torr attained in the tube,

ii. elimination of health harzards associated with handling the expendable tritium target. The assembly is replaced as a unit with the target factory enclosed.

Shielding requirements are therefore dictated primarily by the $H^2(H^3,n)He^4$ reaction. The reaction has its maximum yield of 4×10^{11} neutrons/second for thick targets at accelerating potential of 200 kv. The distribution of neutrons from the target being isotropic.

1.3 Recommended Radiation Level

In order to achieve the objectives of radiation protection, the International Commission on Radiological Protection (ICRP) recommends (ICRP Publication 26, 1977) radiation standards in the form of dose equivalent limits (DEL). The latter are specified numerically in a unit called the 'rem' (Roentgen Equivalent Man). An annual limit of 5 rems for external whole body irradiation is recommended. By whole body irradiation, we mean all of the body is assumed to be immersed in a field of radiation that would be uniform if the body were not present. A derived maximum dose rate of 2.5 mrem/hour will be used in this project. The limit is directly

relatable to the ICRP recommendation if the position of maximum dose rate is occupied for 2000 hours per annum, i.e. 40 hours per week, 50 weeks per annum.

1.4 Thesis Layout

In Chapter Two we will examine what general work has been done in the area of shielding with the aim of finding useful hints for undertaking this particular study. The various methods will be examined under the principal elements of which shielding is composed, namely, the underlying Physics and the shielding methodology.

Chapter Three deals with the theory of the Monte Carlo method. The latter makes use of the idea of "random walk" and the theory of probability to describe the mechanisms of collisions, flight directions and length of mean free paths. In this way the neutron transport history through the shield medium is mathematically simulated.

Chapter Four dwells on the methodology of the computing scheme. Based on a specific source and specific shield, a computer algorithm is established to "play" the Monte Carlo "game". Interaction cross sections and other radiological data are reduced to the form suitable for the computation. The Chapter also discusses the methods by which error is reduced, and by which it is estimated.

Finally, Chapter Five gives the results of the Monte Carlo Program and its reliability is discussed.

Chapter 2

SHIELDING METHODS

The various shielding techniques will be considered under three main headings namely:

i. Point Kernel methods,

ii. Removal - Diffusion theory and

iii. Transport theory methods

2.1 Point Kernel Methods

According to Foderaro (1968) the essence of the Point Kernel Methods can be mathematically expressed as

$$R(\underline{r}) = \int S(\underline{r}')\ K(\underline{r}',\underline{r})d\underline{r}' \qquad (2.1)$$

source

where $R(\underline{r})$ is the response function of a detector at spatial distance $\underline{r}$.

$S(\underline{r}')d\underline{r}'$ is the source strength measured in particles per second in spatial element $d\underline{r}'$ about $\underline{r}'$.

$K(\underline{r},\underline{r}')$ is the response Kernel of a detector at $\underline{r}$ to a unit point source located at $\underline{r}'$. This point response kernel depends on the type of particles, their energy, and the composition of the materials between the source and the detector.

The most widely used approximate kernel concept for representing the attenuation of fast neutrons is

the removal cross-section technique. The basic assumption of the technique is that $K(\underline{r},r')$ is of exponential form i.e.

$$K(\underline{r},\underline{r}') \sim e^{-\Sigma_R|\underline{r}-\underline{r}'|}$$

where Σ_R is the effective macroscopic removal cross section for the shield material.

Various theoretical models have been developed that rely on the removal cross section concept. A notable feature of the models is the different form taken by the removal cross section. This difference arises mainly because the definition of Σ_R is not an intrinsic part of the particular model. The two most commonly used models will be examined briefly.

(a) Albert-Welton Kernel

Albert and Welton (1950) developed a semi-empirical method for calculating neutron attenuation through hydrogeneous shields. The basis of this theory lies in the fact that the collision of a neutron with a hydrogen atom can roughly be equated to an absorption process in thick shields since the average logarithmic energy decrement is large and the rapid increase of the elastic scattering cross section of hydrogen with decreasing neutron energy leads to a rapid moderation. For shielding purposes, inelastic scattering by heavy nuclei likewise has the character of absorption if the shielding medium contains water besides the heavy

material. The attenuating effect of the shield is represented by the various removal cross sections. For hydrogen the removal cross section is taken to be the energy dependent removal cross section. The Albert-Welton expression for the removal component of fast neutrons which penetrate through a mixture of hydrogen and heavy materials from a point isotropic source is given by

$$\phi_R = \frac{K}{4\pi R^2} \int_0^\infty e^{-\Sigma^H(E)R} \, dE \, e^{-\Sigma_i (g_i \Sigma_R^{(i)} R)} \qquad (2.2)$$

where ϕ_R is the total removal flux density at a distance R from the source.

$\Sigma_R^{(i)}$ is the macroscopic effective removal cross section for the i-th heavy element.

g_i is the volume fraction of the i-th non-hydrogeneous element.

$\Sigma^H(E)$ is the total macroscopic cross section for hydrogen.

K is a suitable constant of proportionality.

(b) Spinney Kernel

Spinney (1957) concieved the method which also considers hydrogen as a special case. It predicts the penetration of those neutrons which have had one or more collisions but have suffered only a small angular deflection or insignificant energy loss by means of a simple uncollided point Kernel.

$$\phi_r = \frac{Se^{-\Sigma_r R}}{4\pi R^2}$$

where ϕ_r is the removal flux and Σ_r is the removal cross section. S and R are the source strength and distance respectively

Spinney observed that the removal cross section referred to should be less than the total cross section for a material, and can be expressed generally as

$$\Sigma_r = \Sigma - f\,\Sigma_s$$

where Σ_s is the elastic scattering cross section,
f is the fraction of elastic collisions which can be regarded as glancing,
Σ is the total macroscopic cross-section.

Point Kernel methods are considered unsuitable for this project because, firstly, the methods are based on empirical concepts. The macroscopic removal cross section for a given material can only be deduced experimentally. But no source of 14 MeV neutrons is presently available for such experimental deduction. Secondly, Point Kernel methods are usually applied to fission neutron spectra. For fast neutrons, the expressions are only valid if a minimum of 50 cm of water is placed between the point of interest and the shield material. However, this work intends to use only a single shield material-ordinary concrete. Thirdly, the methods are based on approximate expressions. It is the desire of this project to establish a more reliable technique, based on a rigorous theory.

2.2 Removal Diffusion Theory

One of the most effective of the non-rigorous procedures for solving the problem of the complete attenuation of the neutrons through a shield is the method of combined Removal-Diffusion. This procedure treats the complete attenuation by a combination of two different methods:

i. the behaviour of the penetrative fast neutron beam is described by removal theory which relies heavily on the concept of removal cross-section.

ii. the behaviour of the slowing-down and thermalizing neutrons is described by diffusion theory.

Most combined Removal Diffusion methods in current use are based on the earlier work by Spinney (1957) and later by Avery, et al (1960). It is instructive to focus on the Spinney removal method as described by Avery.

In the Spinney approach, the energy spectrum of neutrons is divided into eight intervals covering the range 0-18 MeV. All neutrons entering the shield are assumed to penetrate initially according to a removal Kernel of the form

$$\phi \sim \int_0^\infty f(E)\, e^{-\Sigma_R(E)R}\, dE \qquad (2.4)$$

where $f(E)$ is the neutron spectrum and

$\Sigma_R(E)$ is the removal cross section.

Neutrons making "removal" collisions are treated as sources for multigroup diffusion calculation.

For most practical applications of the energy dependent diffusion equation it is found convenient to discretize the energy variable E. The effect of discretizing the energy in this way is to replace the energy dependent equation by a set of coupled multigroup equations. Each member of the set can then be treated as a 1-speed diffusion equation for the neutron flux corresponding to the particular group, thereby simplifying the numerical solution of the problem. Gotenhuis and Butler (1956), Ducan (1958) have used this approach to determine the shield dimension for the boiling water test and organic moderated reactors respectively.

If the shielding medium has insufficient moderating power to justify the application of the neutron removal cross section either as the source term of the thermal group in the one-group diffusion theory or in the case of fast neutron shielding, as a means of obtaining a better description of the neutron absorption density, an intermediate group is introduced. Vernon (1950) reported the use of this approach for preliminary calculation of the concrete shield thickness required by a Sodium Cooled Experimental Reactor.

The Removal-Diffusion method can not be used in this project, however, because it is based on empirical concepts.

2.3 Transport Theory Methods

Transport theory methods are based upon, and are identifiable with, the solution of the Boltzmann transport equation. Three methods in particular have proved of greatest importance in shielding studies, these are

(a) Moments method

(b) Discrete-ordinates method, and

(c) Monte-Carlo method

Moments Method

The method, developed by Spencer and Fano (1951), is a semi-numerical theory for solving the Boltzmann transport equation for angle and energy dependent flux in an infinite homogeneous medium.

The theory can be divided into two stages:

i. The angular flux density and source are treated by spherical harmonics, thus the flux becomes, for 1-dimension geometry

$$\phi(x,E\,\mu) = \sum_{\ell=0}^{L} \frac{(2\ell+1)}{2} F_\ell(X,E)P_\ell(\mu) \qquad (2.5)$$

where $\phi(x,E,\mu)$ is the flux density,

$F_\ell(x,E)$ and

$P_\ell(\mu)$ are the spatial and direction coefficients respectively.

ii. The spatial dependence is treated by the moments, $M_{n\ell}$, defined as

$$M_{n\ell}(E) = \frac{1}{2n!} \int_{\infty}^{\infty} X^n F_{\ell}(X,E)dX \qquad (2.6)$$

The spatial distribution is reconstructed from the moments directly or by fitting the moments of the simple functions such as $\exp(-\mu x)$ or $\exp(-(yx)^2)$ to the calculated moments.

Although this technique is applicable to both neutron and gamma rays, it has only been found to be successful in gamma ray build-up factors. However, the practical restriction to an infinite medium due to the difficulty of the spatial reconstruction severely limits the applicability of the moments in shield design.

Discret Ordinates Method

Carlson (1955) introduced the first Discrete Ordinates or Sn method. It has been reviewed by Lee (1962), Carlson (1963), Larthop (1965) and Mynatt (1968).

The Sn method is a numerical technique for solving the finite differenee form of the Boltzmann transport equation. The method may be applied to a spherical geometry by converting the steady state transport equation in spherical geometry into a finite difference equation. In a sphere the phase-space is

$$dVdEd\mu = 4\pi r^2 dr\, dE\, d\mu$$

where dV, dE and dμ are the elements defining volume energy and direction of the phase-space

The finite cell is

$$V_\ell \Delta\mu_m \Delta E_G = \frac{4\pi}{3}(r_{i+1}^3 - r_i^3)(\mu_{d+1}-\mu_d)$$

The volume from r=0 to the outer radius R is subdivided into intervals bounded by the radii r_i. The energy is treated by the multigroup method. The G th group has boundaries E_g, E_{g+1}. Discrete angles are chosen having direction cosines μ_m with m= 1 to n+1. A value of n=8 is most commonly chosen. These directions define the midpoint or average cosine. The solid angles associated with each direction is defined by a corresponding weight w_m. The number and values of μ_m w_m are chosen to meet certain conditions such as accurate representation of the anisotropic angular flux density and accurate integration over the differential scattering cross section. The integration is a numerical quadrature weight w_m. This way the integro-differential equation can be replaced by a series of coupled finite-

difference equation in the discrete spatial co-ordinate r_i, discrete angle $\cos^{-1}(\mu_m)$ and energy integrated group, g. The discrete ordinates are the N_i, m, g, that is the angular flux densities that we want to find.

The scalar flux density $\phi_{i,g}$ is obtained from the relation

$$\phi_{i,g} = \frac{1}{4\pi} \Sigma_m H_{i,m,g}$$

Mynatt (1968) reported the following advantages about the method.

i. Depending somewhat on the sophistication desired, the S_n calculations are easy to prepare.

ii. The method is not stochastic and flux errors at deep penetration are systematic rather than statistical.

iii. Production problems having similar characteristics benefit from fluxes calculated in similar case.

iv. The neutron energy range from higher fission energies to thermal, including up-scattering may be calculated by the same method.

v. The one-dimensional calculations are much faster than similar Monte Carlo calculations.

Its disadvantages were:

i. Convergence of the iterative method is not always uniform and well defined.

ii. Flux abberations are frequently observed in two dimensions due to localized sources and propagation in discrete directions.

iii. The method is not suitable for 3-dimensional calculations for the same reason, and

iv. No basic ground rules exist which define for a particular problem the best direction, set, space, mesh, multigroup and polynomial expansion.

Monte Carlo Method

The Monte Carlo method is an artificial sampling method which can be used for solving complicated problems in an analytic formulation and for simulating purely statistical problems.

The use of Monte Carlo in solving the transport of neutrons may be interpreted in two ways:

Firstly, it is a stochastical method to simulate stochastic processes. Transport of neutrons is characterized by travel along path between widely spaced collision points. On collision, the particles may be absorbed or scattered into a new direction and energy. The Monte Carlo method simulates this behaviour, and then obtains the flux density by averaging the score from thousands of individual particle tracks.

Secondly, Monte Carlo is a stochastic method for solving deterministic problems. The transport of neutrons may be presented as the integral form of the Boltzmann equation

$$F(R) = S(R) + \int K(R' \rightarrow R)F(R')dR' \qquad (2.7)$$

where F(R) is the density of particles in phase-point R

$S(R)$ is the density of particles from source

$K(R' \rightarrow R)$ is the density of particles at R due to a source at R'

Usually in transport calculations we want to estimate the functional quantity λ

$$\lambda = \int h(R)F(R)\,dR \qquad (2.8)$$

where $h(R)$ is the response function. In equation (2.7) $K(R' \rightarrow R)$ may be split into 2 parts

$$K(R' \rightarrow R) = K_m(R' \rightarrow R) + K_n(R' \rightarrow R)$$

The first part describes the multiplying process. It becomes zero in shielding problems. The second part describes non-multiplying transport. Equation (2.7) and (2.8) may be normalized if for all R

$$S(R)\,dR \geq 0$$

$$K_n(R' \rightarrow R) \geq 0$$

and that

$$\int S(R)\,dR = 1,$$

$$\int K_n(R' \rightarrow R)\,dR \leq 1$$

Thus it means that all particles will be ultimately eliminated

We now expand equation 2.7 in finite Neumann series

$$F(R) = \Sigma_v F_v(R)$$

with $F_o(R) = S(R)$ and

$$F_v = \int F_{v-1}(R')\,K(R' \rightarrow R)\,dR'$$

Thus we obtain the Monte Carlo estimates as a sum over discrete contributions

$$\bar{\lambda} = \frac{1}{N} \sum_{i=1} h(R')$$

If N becomes large

$$\lim_{N \to \infty} \bar{\lambda} = \lambda$$

Transport theory techniques, Monte Carlo being one, are sometimes referred to as higher order transport methods, thereby implying that the solutions that they provide are intrinsically more accurate than those obtainable from diffusion theory or Kernel methods. In addition, the Monte Carlo method has the following desirable features suitable for our work which the other transport methods do not.

i. The limited size and speed of the computing machine at our disposal does not enable us to perform an excessively complex process in a practicable time. However, direct analogue technique and application of variance reduction schemes make it possible to obtain reasonable results from Monte Carlo.

ii. Scattering of neutrons in a shield is a three-dimensional process. Therefore in order to adequately account for the contribution of the scattered radiation at a given point outside the shield one must employ a three-dimensional technique. Various authors (Schmidt, 1978, Maienschein, 1970 for example) agree that Monte Carlo is the only rigorous technique available for such task.

iii. In the basic form of the method, the programmer carries out a game or 'experiment' on the computer by simulating the actual physical processes which govern the real particle's behaviour. Thus the physical realism that can be retained in the mathematical formulation makes the scheme easy to handle.

Chapter 3

THEORY

3.1 Neutron Interaction with Matter

In contrast to the interactions of charged particles and gamma rays with matter, which are mainly electromagnetic in nature, and have cross sections that vary relatively smoothly with atomic number, the interactions of neutrons with matter occur mainly through strong nuclear forces. Different but general trends follow mass number due to the charge independence of the nuclear force. Because the range of the nuclear force is about 10^{-12} centimeters, compared with interactomic spacing of about 10^{-8} centimeters, it is expected that the mean free path is of the order of several cm between the nuclear encounters.

The general trend may be summarized as follows:

i. The probability of absorption of neutrons at high energy is much smaller than at lower energies. Consequently neutron attenuation in shields is accomplished by slowing down the neutrons in order that they may be absorbed.

ii. The lower the atomic number of the scattering nucleus the greater the energy loss per collision. Hydrogen, which is far superior to all other elements in this respect, greatly enhances the efficiency of neutron shields by its presence. In deed, the Monte Carlo study of shield pene - tration is implied by a high hydrogen content

because of the regular behaviour of the hydrogen cross section. In the absence of hydrogen, the path of the neutron within the shield becomes much more complicated and the analysis more difficult.

The principal interactions of neutrons with matter in the energy range of interest (i.e. less than 15 MeV) are:

i. elastic scattering (n,n),
ii. inelastic scattering (n, n'),
iii. radiative capture (n, gamma),
iv. absorption with charged particle emission (e.g. (n,p)),
v. fission (n, F), and
vi. (n, 2n) and similar reactions.

3.1.1. Elastic Scattering

A widely used Monte Carlo model for neutron attenuation in shields uses the concept of neutron elastic scattering to obtain a simple relationship between the new energy and the neutron angle of scattering. Elastic scattering is dominant in concrete since it consists, mainly of lighter nuclei. Elastic collisions of neutrons with nuclei are of two types. The one of major interest in nuclear systems is the so-called potential scattering (Profio, 1979); for nuclei of low mass number it occurs with neutron energies up to a few MeV. In this type of scattering there is no compound nucleus formation and scattering results from short range forces acting on the neutron as it

approaches the nucleus. In the other type of elastic scattering known as resonance (or compound nucleus) scattering a compound nucleus expels a neutron leaving the target in its ground state. The end result of these interactions is the same in so far as shielding is concerned and the sum of their cross sections will form the total elastic scattering cross section.

We will examine the elastic scattering of a neutron by a nucleus with mass number A. Such a scattering process is determined by a pair of random variables, which may conveniently be taken as the angle θ of scattering in a system of co-ordinates stationary with respect to the center of mass of the neutron and nucleus, and azimuthal angle χ of scattering:

$$o \leq \theta \leq \pi, \quad o \leq \chi \leq 2\pi$$

The relationship of energy lost by the neutron and the angle through which it scatters is derived in appendix A from considerations of conservation of energy and momentum. The energy after collision, E', is given in terms of the energy before collision, E, by

$$\frac{E'}{E} = \frac{A^2 + 2A\cos\theta + 1}{(A+1)^2} \qquad (3.1)$$

where A is the atomic mass of the scattering nucleus in atomic mass units and

θ is the scattering angle in the center of mass coordinates.

The angle of scattering, ψ in the laboratory system is given by

$$\cos \psi = \frac{A \cos\theta + 1}{(A^2 + 2A\cos\theta + 1)^{\frac{1}{2}}} \qquad (3.2)$$

The probability distribution of the scattering angle varies with the scattering nucleus and with the energy of the neutron. The distribution tends toward isotropy except for very energetic neutrons (Selph, 1968). For hydrogen the distribution is isotropic within a factor of two energies up to about 40 MeV. For heavier elements the practical upper limit is $E = 5 \text{ MeV } A^{-2/3}$. The refraction of the neutrons around the edge of the nucleus produces a forward peak in the distribution which becomes more pronounced with increasing energy. Treatment of direction of scattering in the modelling of neutron history is covered in section 3.2.3.

3.1.2 Inelastic Scattering

This type of scattering is said to occur when a fast neutron is first captured by the target nucleus to form an excited state of the compound nucleus, a neutron of lower kinetic energy is then emitted leaving the target nucleus in an excited state. The excess energy is subsequently emitted as one or more gamma radiations.

It is perhaps instructive to note that another type of inelastic scattering can occur at low neutron energies, generally below a few eV, if the scattering atom (or

nucleus) is not free but is bound in a molecule or in a solid (Selph, 1968; Glasstone and Sesonke, 1981). In the collision of a low energy neutron with a bound scattering atom, there can be a loss or gain of internal energy associated with a change in the vibrational or rotational states. There is no compound nucleus formation in this low energy type of inelastic scattering. This type of inelastic scattering is usually ignored in shielding computations because of the low incident neutron energy involved.

For concrete the inelastic scattering process occurs in all elements except hydrogen. For elements of moderate and high mass number, the threshold energy is usually 0.1 to 1 MeV. With decreasing mass number of the nucleus there is a general tendency for the excitation energy to increase so that the neutrons must have higher energies if they are to undergo inelastic scattering. The threshold for such scattering in oxygen is about 6 MeV and it is 5 MeV in carbon. Inelastic scattering by reducing the neutron energy to a level where it will more readily interact elastically with the light elements.

Inelastic scattering can be isotropic and anisotropic, but it is usually assumed to be isotropic in the laboratory system of coordinates (Profio, 1979). The energy distribution, according to Shreider (1967), is given by empirical or semi-empirical curves. In many cases when the inelastic scattering of neutrons from massive nuclei is being considered, the distribution of the energy E' of the scattered neutron is proportional to

$$E'e^{-E'/T}$$

where $T = a\sqrt{E}$

a is the constant of proportionality depending on the nature of the material

E is the energy before collision, and

$0 \leq E' \leq E$

The formula for E' may be presented in the form

$$1 - e^{-E'/T}(1+E'/T) = \gamma[1-e^{-E'/T}(1+E/T)] \quad (3.3)$$

Equation (3.3) has a unique positive root ε when

$$0 < \varepsilon < 1$$

This root may be computed by an iterative method. If

$$y^{(s)} > 0$$

is arbitrary, then

$$y^{(s+1)} = \ln(1+y^{(s)}) - \ln \varepsilon$$

where s is an integer

3.1.3 Other Interactions

The remaining types of reactions (types iii to vi) are usually grouped and referred to as absorption reactions in Monte Carlo computations. We will discuss their characteristics briefly.

Radiative Capture

Radiative capture of neutrons generally refers to reactions in which a low or intermediate energy neutron is assimilated into the nucleus and no particles are emitted. The compound nucleus formed in this manner has

an excitation due to the neutron binding energy. The excitation energy is released as one or more gamma rays.

This reaction, which occurs in all concrete elements, is the ultimate fate of the neutrons attenuated by the shield. The gamma radiation given off from this interaction is often the major contributor to the radiation dose penetrating a shield because it is highly energetic and is generated throughout the shield (Selph, 1968, Profio, 1979). Some types of concrete used in neutron shielding contain boron to reduce the generation of these penetrating gamma rays.

Charged Particle Emission

Absorption with emission of charged particles such as (n,p) and (n, alpha) reactions, is possible when the excitation energy is sufficient to give a significant probability of penetrating the coulomb barrier. There are no charged particle emitting reactions in hydrogen. In a few light elements of concrete (n,p) and (n, alpha) reactions are exoergic and thus occur even with thermal neutrons. In others the (n,p) and (n, alpha) reactions are endoergic. Therefore charged particle reactions are most prevalent for neutron energies in the MeV range and are characteristic of fast neutron reactions along with inelastic, elastic and other reactions, such as (n, 2n) (Profio, 1979). One of these reactions, $^{10}B(n, alpha)^{7}Li$, is useful for depressing the thermal neutron flux without giving rise to energetic gamma rays.

Fission and Other Reactions

At high energies the excited nucleus remaining after emission of one neutron may emit additional neutrons instead of charged particles or gamma rays, thus (n,2n) and (n, 3n) reactions may occur. As these reactions are always endoergic, they are characterized by a threshold and release a broad spectrum of low energy neutrons. The actual energy spectrum may be known or may be approximated by an evaporation model sprectrum fof the form

$$n(E) = \text{constant } \frac{E}{T^2} e^{-E/T}$$

where n(E) is the number density expressed as a function of the energy variable E, and T is a nuclear 'temperature' expressed in energy units.

It is usually assumed that emission is isotropic in the laboratory system (Profio, 1979 and Shreider, 1967). Shields, however, do not generally contain fissionable materials.

3.2 Modelling of Neutron History

The life history of a neutron is built up from a knowledge of its trajectory through the particular system of interest. In order to track the neutron during its journey we require to know its spatial coordinates (x,y,z); the spherical coordinates (θ,ϕ) of its direction; and its energy E. These variables are sufficient to define the state α, of the particle, where

$$\alpha = \alpha(x,y,z, E,\theta, \phi)$$

A neutron's trajectory from collision to collision can be constructed as a succession of states α_o, α_1, ... α_n, where the i th state is

$$\alpha_i = \alpha_i(x_i, y_i, z_i; E_i; \theta_i, \phi_i)$$

That is, in the i^{th} state, a neutron has the spatial coordinates of the i^{th} collision point and the energy and direction of the neutron after the i^{th} collision. With the exception of the initial state, each successive state is a function of the previous state and the scattering laws governing the neutron in the medium. Thus one could commence with initial, or source conditions, define α_o, choose by random sampling from the relevant probability distributions the new values of the variables which determine α_1 and so on. In this way the individual life history can be constructed.

3.2.1 Direction of Neutron Flight from Source

The neutron generator is a source of isotropic neutrons. Thus the problem is that of choosing a vector at random from a unit sphere in three-dimensional space. As the generator is assumed to be a point source, we use spherical coordinates (θ,ϕ)

$$0 \leq \theta \leq \pi, \qquad 0 \leq \phi, \leq 2\pi$$

as shown in figure 3.1 Cos θ is distributed in the range (-1,1). So is the number $(1-2r_1)$, r_1 being

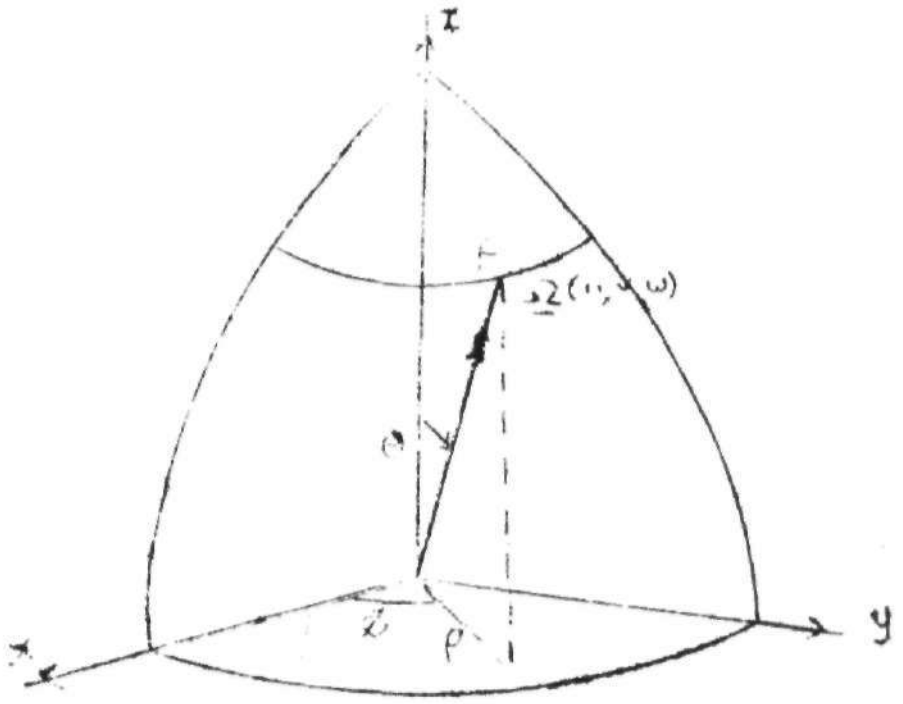


Figure 3.1 - Spherical co-ordinates of a unit vector $\underline{\Omega}$. P is any point on the surface of the unit sphere.

being a random number uniformly distributed in the range (0,1). By the inverse cummulative function method, which states that a random variable from a given probability distribution function can be expressed as a function of another random variable that is uniformly distributed between zero and one (i.e. from the caonical distribution), we may express

$$\theta = \mathrm{Cos}^{-1}(1-2r_1) \qquad (3.4)$$

In the same manner, ϕ is selected uniformly by

$$\phi = \pi(2r_2 - 1) \qquad (3.5)$$

where r_2 is a random variable

The cosines with respect to the x,y,z axis (u,v,w respectively) may be chosen by selecting the point p on the unit sphere

$$u^2 + v^2 + w^2 = 1$$

Referring to figure 3.1, we may put

$$w = \cos\theta = (1-2r_1)$$

and projecting the unit direction vector on the u-v plane the project radius

$$\rho = (u^2 + v^2)^{\frac{1}{2}}$$
$$= (1-w^2)^{\frac{1}{2}}$$

The direction cosines are

$$w = \text{Cos } \theta \quad = (1 - 2r_1)$$

$$u = \rho \text{ Cos } \phi \qquad (3.6)$$

$$v = \rho \text{Sin } \phi, \quad \phi = \pi\ (2r_2 - 1)$$

3.2.2 Length of Mean Free Path

Suppose I(x) is the intensity of the neutrons that have not collided after penetrating the distance x into the shield. Then the decrease in intensity is given by

$$- dI(x) = \Sigma_t I(x)dx$$

or

$$- \frac{dI(x)}{I(x)} = \Sigma_t\, dx$$

Where Σ_t is the macroscopic cross section for all types of reactions.

Since the quantity dI(x) is equally the number of neutrons out of a total of I(x) that collide in dx, it follows that

$$\frac{dI(x)}{I(x)}$$

is the probability that a neutron survives up to x without a collision, interacts in the next dx. In other words the path length, ℓ, or distance to the collision point should be exponentially distributed:

$$P_\ell(x) = \Sigma_t\, e^{-\int_0^x \Sigma_t ds}$$

where s is the distance from the previous collision, along the direction of motion of the neutron.

The probability of the neutron having an interaction at any distance less than x is

$$P(S < x) = 1 - e^{-\int_0^x \Sigma_t ds}$$

In a homogeneous material, for which Σ_t does not depend on s, the average length of a free path is

$$\ell = \Sigma_t^{-1}$$

The length of the free path is simulated thus: If we set a random number, r

$$r = P(\ell < x) = P(L)$$

or $$P(L) = 1 - e^{\Sigma_t x}$$

$$= 1 - e^{L}$$

where $L = \frac{x}{\ell} = \Sigma_t x$

we obtain

$$L = - \ln(1-r)$$

$$= -\ln r$$

because r is distributed in the same way as (1-r). L is also called the physical path length in units of the mean free path.

For a heterogeneous material such as concrete, it may be subdivided into a small number of regions inside each of which the constitution of the material may be regarded as being constant. This can be stated more explicitly by illustrating with a medium that consists of n types of nuclides. Let their cross sections be

$\Sigma_1, \Sigma_2, \ldots, \Sigma_n$ respectively. Let a neutron start from the point $\underline{r}$, and move in the direction of a unit vector $\underline{\Omega}$. The equation of the trajectory (or path) may be written in the form

$$\underline{r}' = \underline{r} + \ell\underline{\Omega}$$

where $\underline{r}'$ is the new position and

ℓ is the path length.

The value of ℓ is obtained from the path length of the i^{th} nuclide, its cross section being Σ_i

$$\ell = \ell_i = - \frac{\ln R}{\Sigma_i}$$

The i^{th} nuclide is chosen if

$$\frac{\Sigma_1 + \Sigma_2 + \ldots + \Sigma_{i-1}}{\Sigma_1 + \Sigma_2 + \ldots + \Sigma_n} < R \leq \frac{\Sigma_1 + \Sigma_2 + \ldots + \Sigma_i}{\Sigma_1 + \Sigma_2 + \ldots + \Sigma_n}$$

where R is a random number

3.2.3 Direction of Scattering

In 1946, Von Neumann and Ulam made the observation that the angular distribution of the scattered neutron as a function of its incident energy and mass of the target nucleus may be divided into three types.

i. Isotropic scattering in the center of mass system. In hydrogen and most other light elements, scattering is isotropic in the center of mass system up to about 10 MeV. Cos θ is therefore distributed uniformly in the interval (-1, + 1) and the angle ϕ is distributed uniformly in the

interval $(0, 2\pi)$. The rule of simulating the scattering is thus:

Find a pair of random numbers r_1 and r_2 and put

$\text{Cos } \theta = 2r_1 - 1$, $\chi = 2\pi r_2$

Then find Cos ψ and E' by means of equations (3.1) and (3.2).

ii. Anisotropic scattering in the center of mass system. This is specially for higher energies and heavier elements. The azimuthal angle χ_1 as before is assumed to be uniform over the range $(0, 2\pi)$. The formula for simulating the variable

$$\mu = \text{Cos } \theta$$

has the form

$$2\pi \int_0^{\mu} \sigma_e(\theta)\, d\mu = r\, \sigma_{se}$$

where $\sigma_e(\theta)$ is the differential elastic saattering cross section in the center of mass system.

σ_{se} is the scattering cross section in the laboratory system, and

r is a random number

From the condition of normality of the probability density function

$$\sigma_e'\theta) = \frac{\sigma_{se}}{4\pi}$$

Substituting we get

$$\mu = (2r - 1)$$

iii. Elastic scattering from a massive nucleus (A)>1).
It follows from equation (3.1) and (3.2) that

$$E' \approx E, \quad \cos\psi \approx \cos\theta$$

Experimental results show that majority of massive nuclei scatter neutrons anisotropically. The corresponding differential scattering cross section is therefore not constant. However in our computations we will neglect the effect of elastic scattering in type iii, since most concrete nuclides are rather light nuclides.

Hence in calculating the direction, based on the foregoing discussion, we may generally assume that light nuclei on one hand, scatter isotropically in the center of mass system, and heavy elements in the laboratory system (cf. Lu and Bull, 1972).

If a unit vector in the direction of the velocity of a neutron before scattering is denoted by $\underline{\Omega}$ then in cartesian coordinates

$$\underline{\Omega} = u\underline{i} + v\underline{j} + w\underline{k}$$

$$u^2 + v^2 + w^2 = 1$$

A unit vector in the direction of the velocity of the neutron after scattering is denoted by $\underline{\Omega}'$ and its coordinates are denoted by u', v', w', θ'. ϕ'.

(i) Isotropic scattering in the center of mass system

The expressions for the new coordinates in terms of the old may be written as

$$w' = w \cos\psi + \sin\psi \cos\chi \,(1-w^2)^{\frac{1}{2}}$$

$$v' = \frac{1}{1-w^2}\left\{ v(\cos\psi - ww') + \sin\psi \sin\chi\, u(1-w^2)^{\frac{1}{2}} \right\} \quad (3.7)$$

$$u' = \frac{1}{1-w^2}\left\{ u(\cos\psi - ww') - \sin\psi \sin\chi\, v(1-w^2)^{\frac{1}{2}} \right\}$$

ii. Isotropic scattering in the laboratory system of coordinates.

According to Shreider (1967), the new direction $\underline{\Omega}'$ does not depend on $\underline{\Omega}$. It is convenient to simulate it thus:

1. Take a random number r and put

$$\cos\theta' = 2r-1$$

2. Take two random numbers r_1 and r_2. If

$$(2r_1 - 1)^2 + r_2^2 \geq 1$$

then the pair is rejected and another pair is taken. If

$$(2r_1 - 1)^2 + r_2^2 < 1$$

then

$$\cos\phi' = \frac{(2r_1 - 1)^2 - r_2^2}{(2r_1 - 1)^2 + r_2^2}$$

$$\sin\phi' = \frac{2(2r_1 - 1)\, r_2}{(2r_1 - 1)^2 + r_2^2}$$

In Cartesian coordinates

$$w' = \cos\theta'$$

$$v' = (1-\cos^2\theta')^{\frac{1}{2}} \sin\phi' \quad (3.8)$$

$$u' = (1-\cos^2\theta')^{\frac{1}{2}} \cos\phi'$$

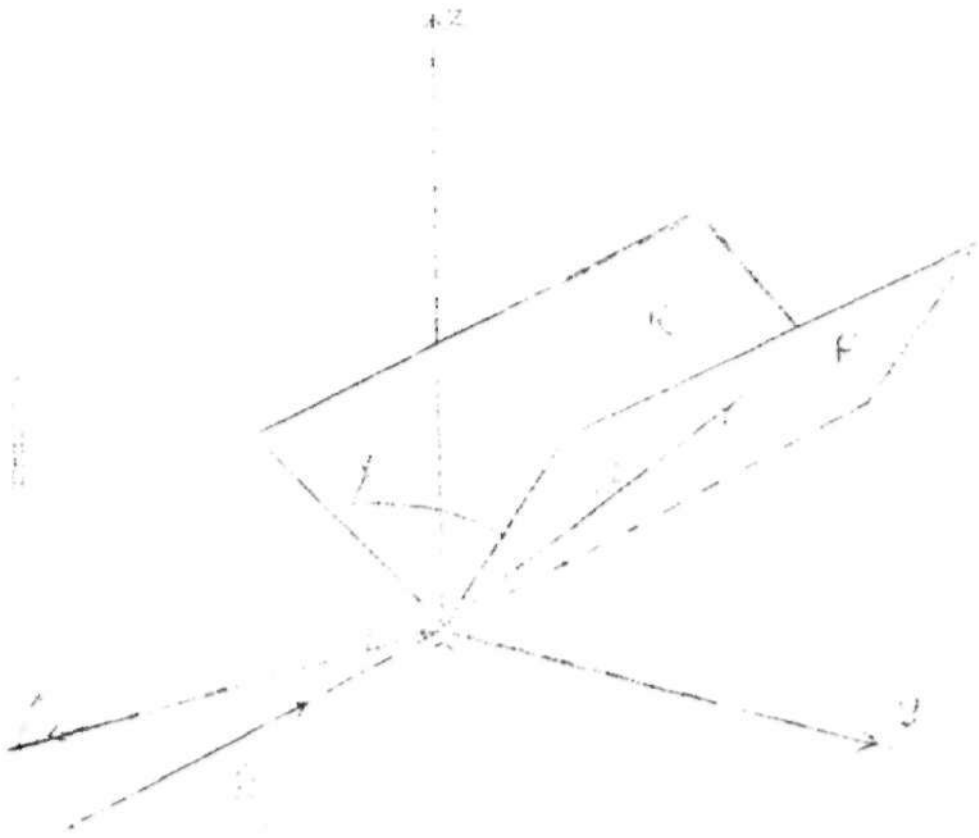


Figure 3.2 - Diagram showing scattering vectors $\bar{\Omega}$ and $\bar{\Omega}'$, where P is the plane of scattering passing through the vectors $\bar{\Omega}'$ and $\bar{\Omega}$. The plane R passes through the axis oz and $\bar{\Omega}$, and the angle χ is the angle subtended by plane P and R at 0 (Shreider, 1967)

Chapter 4

COMPUTER IMPLEMENTATION

4.1 General Description

In writing a Monte Carlo program it is useful to distinguish between two techniques. The strongly physically directed tracking technique, or the direct analogue Monte Carlo, and the non-analogue approach in which the simulation is modified to improve statistical efficiency, and the pseudo-particles are no longer the direct counterparts of the real particles. Various authors are divided on the better approach. For example, Maienschein et al (1970) and Butler (1970) find the direct analogue calculations impractical. They therefore suggest that in developing a Monte Carlo program major effort should be directed toward focussing attention on the important particles by biasing the selection of the samples. Whereas, Devillers, et al (1970), Lu and Bull (1972) and Schnier (1970) favour the direct analogue approach. They criticise the statistical techniques on the ground that they can be misleading.

However, in the present work emphasis is placed on the straight forward direct analogue technique because the non-analogue approach also necessitates a number of trial runs. This calls for a good deal of skill and experience in order to guess some aspects of the solutions. The process starts by selecting a neutron from the spectrum

and ends when the neutron is lost (absorbed by or escape(d) from the medium system. This is analogous to one neutron life cycle. The procedure is as follows (see appendix B for program).

1. Under "source", the program assigns initial coordinates, x,y,z direction cosines, u,v,w; and energy, E to the particle. We may describe the source by separation of variables

$$\alpha(x,y,z,u,v,w,E) = A\, s(x,y,z)q(u,v,w)P(E)$$

We will consider the tritium target of the generator to be a point source, located at the center of the spherical shield. Hence the spatial distribution of the neutrons may be expressed simply as

$$s(x,y,z) = s(o,o,c)$$

Also, the neutrons produced are monoenergetic, and have a uniform angular distribution in the laboratory system. Thus

$$P(E) = P(E_o), \quad E_o = 14.3 \text{ MeV}$$

The treatment of the direction cosines (u,v,w) is discussed in section 3.2.1.

2. The next step is to compute the path length or distance to the first (or next) collision. This step is captioned "path length". Subroutine "select" is built on the guideline of section 3.2.2, to handle neutron flight in a heterogeneous medium. The medium is ordinary concrete which has 10 nuclides. The subroutine begins by taking a random number R from a random sequence. The i^{th} nuclide is chosen if

$$\frac{\Sigma_1+\Sigma_2+\ldots+\Sigma_{i-1}}{\Sigma_1+\Sigma_2+\ldots+\Sigma_{10}} \leq R < \frac{\Sigma_1+\Sigma_2+\ldots+\Sigma_i}{\Sigma_1+\Sigma_2+\ldots+\Sigma_{10}}$$

where Σ_i is the total macroscopic cross section of the i^{th} nuclide.

A new weight is then assigned to the particle. The cross section and mass number of the chosen nuclide are also assigned by the subroutine. Subroutine "Path" is only called to compute the path length and assign new spatial coordinates to the particle if its new weight and energy are not less than the cut-off weight and cut-off energy respectively. If they are, the history is terminated and a new particle is initiated.

3. The "geometry" step determines if an outer boundary is crossed. If it is, the program advances to "score". If not, the program moves to "collision".

4. At "collision" the particle eventually makes a collision. Subroutine "scatter" is called to select the angle of scattering with the aid of random numbers, computes the scattered energy and transforms the direction as discussesd in section 3.3.3. The program then returns to "path" and the history is continued.

5. The step labelled "score" decides if the neutron is "slow","intermediate" or "fast" - depending on the energy. It then tallies the score and records the particle's contribution to the quantities of interest. Another source particle is initiated. If all source particles have been processed the program advances to "output".

6. In "output", the transmission coefficients for "slow", "intermediate" and "fast" neutrons are normalized over the total number of source particles generated. The equivalent flux is computed from the relation:

$$\phi = \frac{\phi_o T}{r^2}$$

where T is the transmission coefficient,

ϕ_o = the initial flux (at 1 cm)
= $\frac{4x10^{11}}{4\pi}$ neutrons/sec-cm^2,

r = shield radius (in centimeters), and

ϕ is the flux at the shield boundary (/sqcm-sec)

The equivalent dose is calculated from the expression

equivalent dose (mrem/h)	=	equivalent flux (/sqcm-sec)	x	conversion factor (mrem/h)/(neutron/sec cm^2)

The conversion factor values are obtainable from ICRP publication 26 (1977). The conversion factor for "slow," "intermediate" and "fast" neutrons is approximated to 0.003, 0.004 and 0.050 (mrem/h)/(neutrons/sqcm-s)respectively.

4.2 Variance Reduction Procedure

The law of large numbers tells us that we may write our Monte Carlo results as

$$\bar{x} \pm \frac{\sigma}{N^{\frac{1}{2}}} \qquad (4.1)$$

where $\bar{x}$ is the mean score of independent variables, x,

$$\sigma = (\bar{x}^2 - (\bar{x})^2)^{\frac{1}{2}}$$

is the standard deviation of individual samples

and

N is the number of particles processed.

It is obvious from equation (4.1) that we could reduce the error by either increasing the number of particles studied or by altering the schematization of the problem so that σ is reduced, but the meaning of $\bar{x}$ remains the same. The method by which the magnitude of N is increased gets to a point at which unacceptably large computing times are required. Thus a more practical alternative is to reduce the variance or σ.

The only strategem currently being incorporated into direct-analogue Monte Carlo is the method of survival weights. With the introduction of weights the program does not allow the absorption of neutrons, as such, all collisions are forced to be scatterings. In subroutine "select" the effect of absorption is accounted for by modifying the weight (initially it is 1.0). The particle's weight after collision is the weight before collision multiplied by the survival probability after collision (i.e. ratio of scattering cross section to the total cross section). With the introduction of this scheme, it is necessary to establish additional criteria for terminating a life history which is to "kill" when its weight becomes less than a cut off weight.

There is no strict mathematical basis for the introduction of weights. But it is intuitively obvious

that it would be more efficient to follow only those particles that experience only scattering collisions; since these have the best chance of ultimately penetrating the shield. The effect is that the result is sampled from many more neutrons, each of lower weight, which should reduce the variance while leaving the mean score unchanged.

4.3 Description of Neutron Cross Section Data

In considering the applicability of the Monte Carlo procedure it is most important to obtain a reliable cross sectional data. Because of the irregular dependence of the neutron interaction cross sections on their energies, most shield designers rely heavily on evaluated values. Plots and references for measured neutron cross section and similar references are compiled in the "barn book" or data files prepared at centers such as the UK Nuclear Data Library. However, measured nuclear data are still as Profio (1979) puts it, "incomplete, imprecise, or disordant" for many nuclides and energies. The data must hence be evaluated to select the best fit, decide between conflicting measurements and fill in the gaps.

Many radiation transport computer programs use the multigroup approximation in which the continuous variation of the cross section with energy is replaced by weighted mean over the interval E_1 to E_2

$$\bar{\sigma}\ (E_1, E_2) = \frac{\int_{E_1}^{E_2} \sigma(E)\ w(E)\ dE}{\int_{E_1}^{E_2} w(E)\ dE} \qquad (4.2)$$

Nuclide	$\bar{\sigma}$ (barns)						
	Slow (0.0001-1eV		Intermediate (1eV-1000eV)		Fast 1keV - 20 MeV		
	$\bar{\sigma}_n$	$\bar{\sigma}_\gamma$	$\bar{\sigma}_n$	$\bar{\sigma}_A$	$\bar{\sigma}_n$	$\bar{\sigma}_A$	$\bar{\sigma}_{n'}$
Al	1.4	0.2	2.3	0.18	2.9	4.8m	0.29
Si	2.1	0.16*	2.5	0.101*	3.0	9.3m	0.15
Mg	1.7	11.7	5.1	1.4	2.8	5.8m	0.92
Fe	11.3	2.26	10.3	1.28	2.5	7.9m	0.62
Ca	7.0	3.3	8.4	4.1	2.9	28m	0.74
		$\bar{\sigma}_A$				$\bar{\sigma}_\gamma$	
H	45.3	0.294	17.2	0.1413	4.0	0.039m	0
C	4.69	3.0m	4.42	1.5m	2.361	0.06m	0.011
O	3.35	0.28m	3.74	0.13m	2.8	7.1m	3.2
Na	3.3	0.47	8.8	0.31	3.18	2.1m	0.48
K	2.2	1.3	2.2	120	2.70	0.1	0.10

Table 4.1 Value of cross sections from UK Nuclear Data Library except values marked *, which are recommended cross sections from 1969 IAEA fit (G.C. Hanna et. al., Atomic Energy Review 7, No. 4, P. 3).

m indicates that cross section is in mb

$\bar{\sigma}_n$ is referred to as the average cross section o if the nucleus remains in the ground state after the interaction.

$\bar{\sigma}_{n'}$ is the cross section if it is left in an an excited state

$\bar{\sigma}_\gamma$ is the radiative capture cross section

$\bar{\sigma}_T$ is the total cross total cross section for all events

such that $\sigma_A = \sigma_T - \sigma_n - \sigma_{n'}$, the absorption cross section

where w(E) is the weighting factor.

A common structure for group cross sections uses equal lethargy intervals. Because too much computer storage and time are required to perform calculations with many groups, it is desirable in this work to reduce the set to a fewer broad group cross sections.

For many elements, an examination of the group reveals the existence of three regions. There is firstly a low energy region, where the cross section decreases steadily with increasing neutron energy. The cross section varies (approximately) inversely as the square of the energy. The average cross section can be shown to be (see Kaye and Laby, 1975):

$$\sigma(E) = \sigma_o \left(\frac{\pi T_o}{4 T_n} \right)^{\frac{1}{2}}$$

where T_n is the temperature of the surrounding and

σ_o is the cross section corresponding to an energy

$$KT_o,\ T_o = 294\ K$$

The integrations in equation (4.2) were taken over the range 0 0001 eV to 1eV, although most of the contribution comes from a narrower range around 0.025eV.

Following the v^{-1} region (or $E^{-\frac{1}{2}}$), the elements exhibit a resonance region usually for neutrons of roughly 0.1 to 1 keV energy. This region is characterized by the resonance of peaks where the cross section rises fairly sharply to high values for certain neutron

energies and then falls again. The average cross section is equal to

$$\bar{\sigma}\ (E) \quad = \quad \frac{\int_{E_1}^{E_2} (\sigma/E)\ dE}{\ln(E_2/E_1)}$$

The numerator is referred to as resonance integral since it gives cummulative absorption cross sections in the various resonances as the neutron slows down from energy E_2 to E_1. Table 4.1 shows values for E_1 = 0.55eV and E_2 = 2MeV although the values are usually insensitive to the upper limit.

At higher energies, apart from resonances, neutron cross sections decrease steadily with increasing neutron energy. The cross sections can be averaged over a neutron spectrum which conventionally is expressed as

$$\phi \quad = \quad \frac{E}{b^2}\ e^{-E/b}$$

where b = 2.0 MeV.

In the table (table 4.1) the average values have been taken over the range 1 KeV to 20 MeV, although most of the contribution comes from a much narrower range around 2 MeV.

4.4 Estimation of Accuracy

Let x_i be the value of the state variable in the process we are modelling for each N independent tests. We assume that this variable has a finite mathematical expectation (usually called the true mean) 'a' and a

variance σ^2. Then its arithmetic mean

$$\bar{\bar{x}} = \frac{\Sigma x_i}{N}$$

is approximately the value of the true mean 'a'. The quantity $\bar{x}$ is the result of the solution of the problem by the Monte Carlo method. The difference between this quantity and the required mathematical expectation, $|\bar{x} - a|$ is the error of the method.

An estimation of the error of the method δ, follows from Chebyshev's inequality

$$\delta = |\bar{\bar{x}} - a| \leq \sigma \sqrt{\frac{1}{\varepsilon N}} \qquad (4.3)$$

where $1 - \varepsilon$ is the certainty of the estimation. In order to make the inequality in equation (4.3) more precise, we denote that the variable $\bar{x}$ is sampled over a large number of independent random variables. Therefore the law of distribution of the variable $\bar{x}$ may be found from the Central Limit Theorem. The theorem states that the variable $\bar{x}$ is distributed almost according to the Gaussian law if the quantity

$$\frac{b}{\sigma^3}, \quad \frac{1}{N^{\frac{1}{2}}}$$

is sufficiently small, where b is the so-called third moment of the variable x_i. Since large values of N are usually used in the Monte Carlo method, then Gauss's law is usually applicable. The Gaussian distribution function

$$P(\bar{x} < T) \sim \phi\left(\frac{T - \bar{x}}{\sigma}\right)$$

where

$$\phi(T) = \frac{1}{(2\pi)^{\frac{1}{2}}} \int_{-\infty}^{T} e^{-t^2/2} dt$$

enables us to estimate the probability of the deviation of $\bar{x}$ from its true mean 'a'. We will take an arbitrary degree of certainty, p. Let T_p be the root of the equation

$$2\phi(T_p) - 1 = P(\bar{x} < T)$$

The probability of the inequality in equation 4.3

$$\bar{x} - a \leq T_p \sigma$$

is approximately equal to p

It is frequently recommended that Tp should be taken as 3 which corresponds to p >0.99. But such an estimate is too excessive in practice. Therefore Wood (1982) and Shreider (1967) suggest a 50% degree of certainty. The probable error is thus defined as

$$\delta = 0.675 \sigma$$

such that the inequalities

$$|\bar{x} - a| < \delta, \quad |\bar{x} - a| \geq \delta$$

are equally probable.

Ordinarily it is rather difficult to estimate the variance σ^2, prior to solving the problem. When solving a specific problem a statistical estimate of the variance is obtained during the process as an estimate of the error

In order to do this, it is sufficient to compute the squares x_i^2 together with the x_i and then

$$\sigma^2 = \frac{1}{N-1}\left[\sum_{i=1}^{N} x_i^2 - N(\bar{x})^2\right]$$

since σ^2 is not required with great accuracy we may use the simpler formula

$$\sigma^2 = \frac{1}{N}\sum_{i=1}^{N} x_i^2 - \left(\frac{1}{N}\sum_{i=1}^{N} x_i\right)^2,$$

for large N(see the corresponding computer program in appendix c).

Chapter 5

DISCUSSION

5.1 Results

Two programs - one to calculate, primarily, the dose rate at the shield boundary, and the other to estimate the corresponding error - were compiled and executed for 1000 neutron histories (see appendix B and C respectively). The output table is shown in appendix D. Figure 5.1 shows a curve of neutron dose rate as a function of the shield thickness.

A derived dose rate limit of 2.5 mrem/h was adopted based on ICRP recommendation (see section 1.3). The curve (Fig.5.1) therefore shows that the thickness required for an ordinary concrete shield surrounding the neutron generator (Energy = 14.3 MeV, flux = 4.0×10^{11} neutrons/second) should be about 2.3 m. The composition of the ordinary concrete material as used in this program is defined in appendix E.

The corresponding statistical error was estimated by assuming an exponential form for the curve in the region around r = 2.3 m, i.e.

Dose,

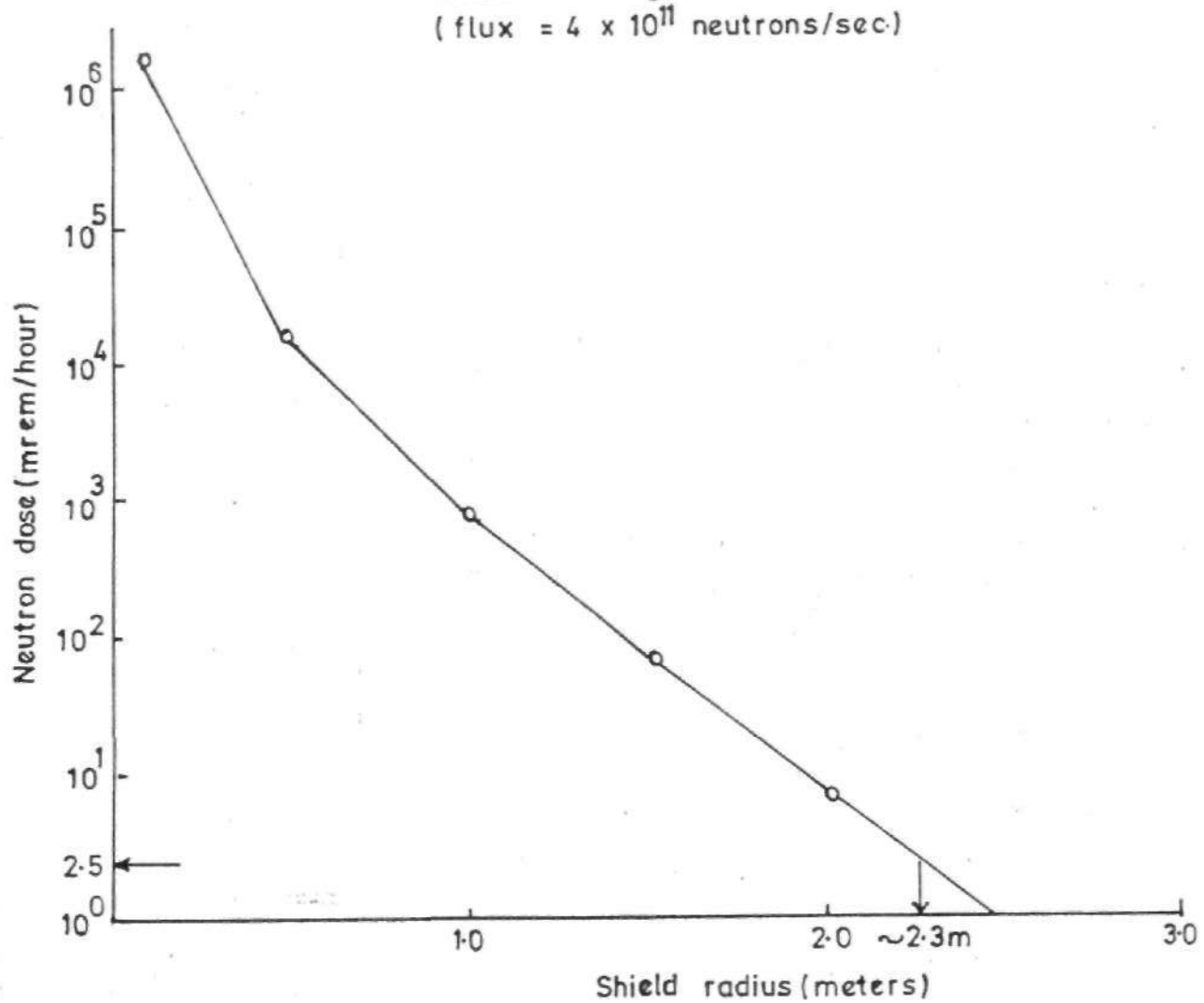
$$D \sim e^{-kr}$$

which implies that

$$\frac{\Delta D}{D} = - k \Delta r$$

this justifies the following approximate relation

Figure 5·1: Estimate of the dose rate outside an ordinary concrete shield enclosing a source of 14·3 MeV neutrons (flux = 4 x 10^{11} neutrons/sec.)



$$\text{Error in } r \equiv \left[\frac{\text{relative error of the dose rate}}{K}\right]$$

K being the slope of the curve. A value of about 0.2 m (about 10% relative error) was thus obtained as error of the program.

Source	Recommended Shield Thickness
NBS Handbook 63 (1957)	2.2 meters
ORINS (1963)	2.6 meters
Present Work	2.3 ± 0.2 m

Table 5.1 - Summary of results obtained by various sources

5.2 Limitations of this work

a. Inaccuracy of cross section values used

Because of the irregular dependence of the neutron interaction cross sections on their energies most Monte Carlo procedures rely heavily on evaluated values. However, Profio (1979) cautions that such data are still incomplete, imprecise and disordant. In the multigroup approximation the continuous variation of the cross section with energy is replaced by a weighted mean. But one of the difficulties which arise when cross sections are averaged is that this yields a large fractional error - sometimes up to 20%.

Another problem is, a weighting spectrum may not give the correct spectrum shape within a group when it comes to averaging over resonances. This problem is difficult to solve even with very fine group cross section. Moreover, not all elements show the type of behaviour described in section 4.3. For example for light nuclides at low energies scattering is dominated by potential scattering and the cross section tends to be independent of energy. Departures also arise at low energies in crystalline materials where the neutron wavelength is comparable to the lattice spacing; and in molecular compounds where collision energy is comparable to the vibrational quanta of the molecular oscillations.

b. Difficulty in estimating the error

In Monte Carlo computations precise error estimates are generally impossible. The accuracy of a complicated calculation is judged according to various supplementary considerations. Such criteria may be provided by the law of large numbers which tells us that a Monte Carlo result converges to the true mean as the number of particles increases. However, in order to obtain more specific information about the accuracy of our calculations, we must turn to the Central Limit Theorem. The latter states that the probability, p, that the exact or true value

of the mean lies in the interval $(\bar{x} - T_p\sigma, \bar{x}+T_p\sigma)$ is equal to $2P(T_p)-1$, where $P(y)$ is the normal cummulative distribution function if the number of samples is large. $\bar{x}$ is the calculated mean. The probable relative error is then given

$$\text{Error} = \frac{0.63}{\bar{x}} \left(\frac{\text{Variance}}{N}\right)^{\frac{1}{2}}$$

where N is the number of histories (section 4.4).

Strictly speaking the Central Limit Theorem refers to the true standard deviation of the sampled population. But in practice, an estimate of this quantity is calculated and used to determine the estimated error. Moreover, the theorem is based on independent samples, but Monte Carlo procedures do not guarantee this.

c. Inadequacy of the Scattering Model

The treatment in subroutine "scatter" (see appendix B) is a neutron elastic scattering process, which assumes that when the neutron scatters it does so in a manner which can be regarded as isotropic in the center of mass coordinate system (for Atomic Mass $\leq$ 16), or isotropic in the laboratory system (for Atomic Mass $>$ 16). Even though this treatment may appear simplistic, similar models of neutron interaction are widely used in Monte Carlo calculations (Wood, 1982; Lu and Bull, 1970). The limitations of the model we have adopted are, namely

(i) The assumption that the target is at rest

Below 1eV, a different scattering model is necessary-one which makes allowance for the kinetic motion of the target atoms, and also takes into account the fact that the struck nucleus is not free to recoil, due to chemical binding effects of the atom in a molecule or a crystal lattice. But to follow by Monte Carlo method the histories of neutrons bearing high energies (14 MeV) to their eventual death by absorption as themal neutrons would entail excessively large computing times, if two different sets of scattering models are used. For this reason, this Monte Carlo model was confined to the stages of the fast neutron's slowing down career.

(ii) The Neglect of Inelastic Scattering Process

It is evident from table 4.1 that for fast neutron attenuation calculations the inelastic scattering process should not be neglected, particularly, for the heavy nuclides present. It was, however, inevitably neglected due to incomplete information regarding the scheme for simulating the scattering (see Section 3.3.2).

5.3 Compensating for Secondary Radiations

Up to this point our calculations have been confined to the attenuation of the primary radiation - the neutrons. In the process of attenuating the fast neutrons by the shield other radiations are inevitably produced, particularly gamma rays.

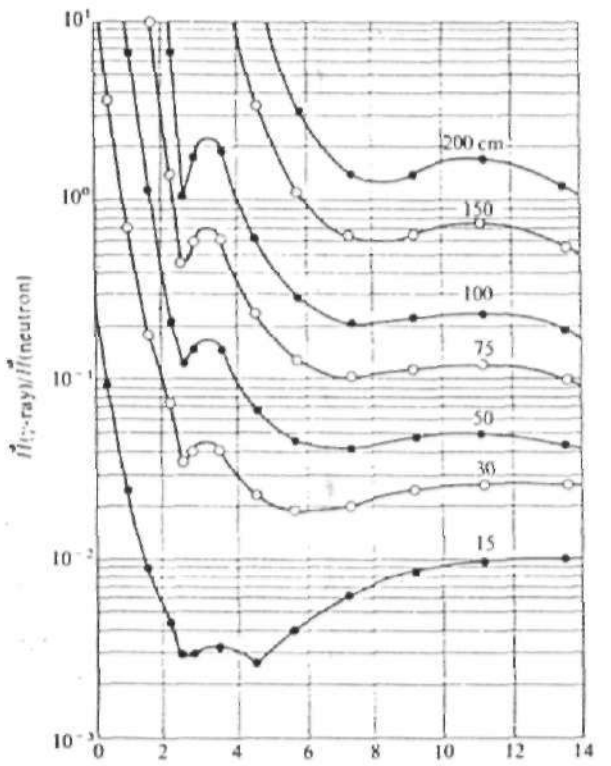


Figure 5.2 Ratio of gamma ray dose to neutron dose for neutrons incident on slabs of concrete, based on Q = 10 for neutrons. (From Clark, F.H. et al, ORNL - 3826, 1966).

Regarding other possible forms of secondary radiation, like alpha-particles and beta-rays, it is not necessary to shield against them because their ranges are short. Table 5.2 summarizes gamma ray energies encountered in neutron capture for concrete shield. Despite efforts being made in recent years there is no accurate theoretical treatment - Monte Carlo or otherwise - of the secondary gamma rays. This is due to the complexity of the radiation spectrum within the shield.

Target	Cross Sections (barns)	Highest energy γ-ray (MeV)	Average Number of Photons per Capture
Al	0.215	7.724	2
O	-	-	-
Si	0.160	10.55	V.L
Fe	2.43	10.16	1.7
Ca	0.406	7,83	1.7
C	0.0045	4.95	V.L
Na	0.47	6.41	1.3
K	1.89	9.2?	< 2
H	0.330	2.230	V.L
Mg	0.059	9.216	V.L

V.L. = Very low

Table 5.2 Gamma rays from thermal neutron capture in ordinary concrete elements (taken from Hittelman, O.S. and Liedtke, R.A., Nucleonic 13 No. 5, 50-51, 1955)

From figure 5.2 the ratio of the dose rate from gamma rays produced in slabs of concrete to the dose rate from neutrons that have penetrated the slabs is shown for various slab thicknesses and as a function of the energy of the incident neutrons. It will be observed that with an incident beam of 14 MeV neutrons, the gamma ray and the neutron dose rates are about for 200 centimeters slab. Thus it would probably be accurate to assume that the 2.3 meters sheild thickness calculated for the neutron attenuation is adequate for attenuating the gamma rays also. In any case, if the otherwise is feared, boron which has a large gamma absorption coefficient (3,900 b) may always be added in the form of boron compounds such as colemanite, boron frits or glass.

5.4 Conclusion

A remarkable aspect of the Monte Carlo method is the little time, effort and cost it takes to estimate shield thicknesses, when compared with the elaborate apparatus needed to undertake the study by most other methods. This work also demonstrates the ease with which calculations may be made in three dimensional geometries. This is one area of shielding calculations in which the Monte Carlo method has not been rivalled by other methods.

Granted, the calculational procedure has suffered major simplifying assumptions such as the

use of highly approximate cross section values and inaccurate scattering model. These steps were taken largely to reduce computing time.

This work recommends a thickness of 2.3 meters for an ordinary concrete material to encase the fast neutron generator under consideration. A maximum statistical error of 10% was obtained for this value. Systematic errors are also envisaged for the calculation, coming from assumptions mentioned above and also discussed in section 5.2.

Another important consideration not covered by this work is the rapid loss of water at temperatures above 90°C (heat generation rate of 0.8 m W cm^{-3}, or temperature rise of 6°C cm^{-3}), since neutron attenuation is governed mainly by the hydrogen - hence water - concentration. Even at low temperatures there is a gradual loss of water. Profio (1979) recommends that to allow for this, the shield thickness should be increased by about 12%.

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APPENDIX A: SCATTERING ANGLE AND SCATTERING ENERGY OF A NEUTRON UNDERGOING ELASTIC COLLISIONS

We shall consider by means of the laws of classical mechanics, based on the principles of the conservation of kinetic energy and momentum, the elastic scattering of a neutron by a nucleus with mass number A. Such a scattering is determined by the angle of scattering θ in a system of co-ordinates stationary with respect to the center of mass of the neutron and nucleus and the azimuthal angle of scattering, χ

$$0 \leq \theta \leq \pi , \qquad 0 \leq \chi \leq 2\pi$$

The conditions before and after a collision as represented in the laboratory and center of mass systems, are shown in figures A.1 and A.2.

The neutron, having a mass of approximately unity on the conventional atomic mass scale, moves with a speed v, relative to the nucleus of mass number A. The speed v_m of the relative center of mass in the laboratory system is given by

$$v_m = \frac{v_1}{A+1} \tag{A.1}$$

In the center of mass system, the velocity of the neutron before collision is $v_1 - v_m$ or from equation (A.1).

$$v_1 - v_m = \frac{Av_1}{A+1} \tag{A.2}$$

Following the collision, if V_a is the speed of the neutron and v_b that of the nucleus after collision in the center of mass system, then conservation of momentum requires that

$$V_a = Av_b \qquad (A.3)$$

The conservation of energy in the center of mass system may therefore be written as

$$\tfrac{1}{2}\left(\frac{Av_1}{A+1}\right)^2 + \tfrac{1}{2}A\left(\frac{V_1}{A+1}\right)^2 = \tfrac{1}{2}v_a^2 + \tfrac{1}{2}Av_b^2$$

Upon solving (A.3) and (A.4) for v_a and v_b we get

$$v_a = \frac{Av_1}{A+1} \quad ; \quad v_b = \frac{v_1}{A+1} \qquad (A.5)$$

In order to determine the loss of kinetic energy of the neutron after collision with an essentially stationary nucleus, it is necessary to transform the results obtained for the center of mass back to the laboratory system.

Now, the final velocity of the neutron after collision in the laboratory system is obtained by adding the vector $\underline{v}_m$ to $\underline{v}_a$. The vector addition is shown in Figure A.3.

Let v_2 be the velocity the neutron has in the laboratory system after collision. The energy, E' it retains is obtained by applying the cosine rule on figure A.2

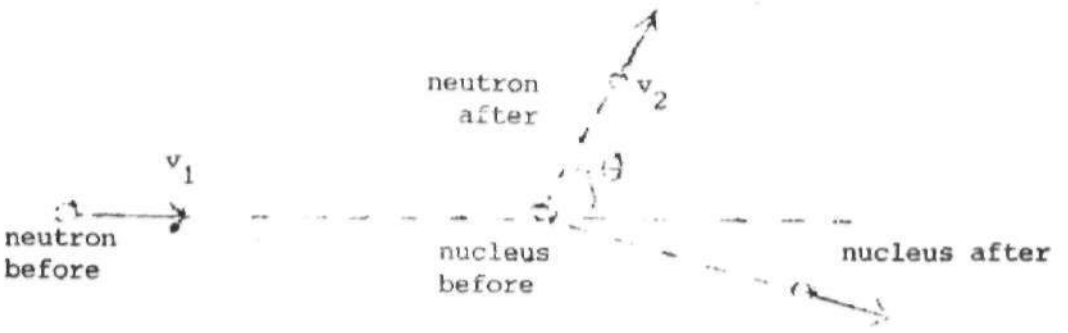


Figure A.1

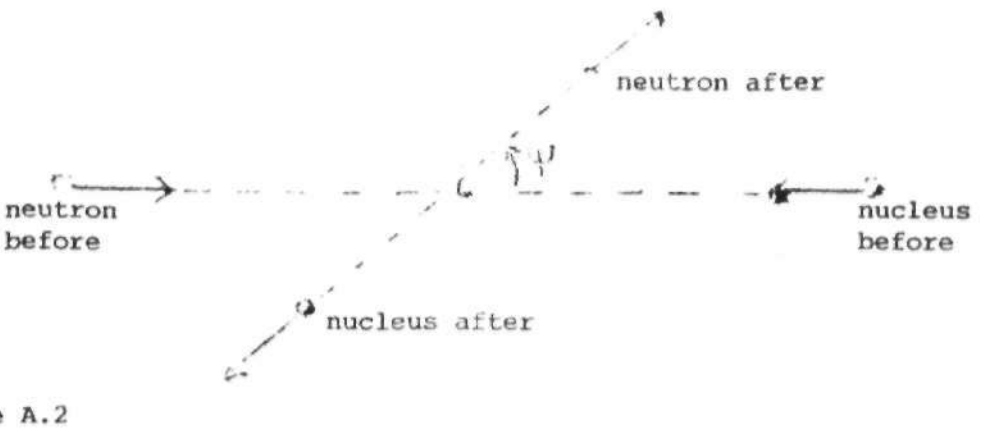


Figure A.2

Figures A.1 and A. 2 show neutron scattering in laboratory and center of mass systems respectively.



Figure A.3 Transformation of center of mass system to laboratory system.

$$v_2^2 = v_m^2 + v_a^2 - 2v_a v_m \cos\theta$$

Substitute for v_m and v_a from equation (A.1) and (A.5)

$$v_2^2 = \frac{v_1^2}{A+1} + \frac{Av_1^2}{(A+1)^2} + \frac{2Av_1^2 \cos\theta}{(A+1)^2}$$

Therefore

$$\frac{E'}{E} = \frac{v_2^2}{v_1^2} = \frac{1 + A^2 + 2A\cos\theta}{(A+1)^2} \qquad (A.6)$$

The angle through which the neutron is deflected from its initial direction, ψ appears in the expression equating velocities along the initial flight direction

$$v_2 \cos\psi = v_a \cos\theta + v_m$$

Again substitute for v_m and v_a we get

$$v_2 \cos\psi = \frac{v_1}{A+1}(1 + A\cos\theta)$$

substituting v_2 we get

$$\cos\psi = \frac{1 + A\cos\theta}{(1+A^2+2A\cos\theta)^{\frac{1}{2}}} \qquad (A.7)$$

APPENDIX B: COMPUTER PROGRAM TO ESTIMATE THE DOSE RATE OUTSIDE A SHIELD.



PROGRAM SHIELD Contd.

```
C     [illegible]

      [illegible]
      [illegible]
      [illegible]
```

PROGRAM SHIELD Contd.

```
      SUBROUTINE PATH(X,Y,R,T,IC,ES)
      A=3.E-4
      B=4.78*(R/.65)
      M=M-1.0
      X=-0.5
      Y=-0.5
      RETURN
      END

      SUBROUTINE SPATT(X,Y,R,T,IC,ES)
      A=3.E-4
      B=4.78*(0.0
      X=-0.5
      Y=-0.5
      IF(R.GT.0.5)GO TO 2
      T=2.0*ASIN(0.5/R)
      GO TO 3
    2 T=2.0*ASIN(0.5/R)
      IF(R.GT.0.5)GO TO 4
      ES=1.0-T/(2.0*3.14159)
      GO TO 5
    4 ES=(R-0.5)*T/(2.0*3.14159)
    5 RETURN
      END
```

APPENDIX C: COMPUTER PROGRAM TO ESTIMATE THE SATISTICAL ERROR OF THE MONTE CARLO CALCULATION

```
      PROGRAM ESTERR(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)
      DIMENSION SS(10),SI(10),SF(10),PA(10),PF(10),AV(10),
     * SSS(10),SII(10),SFF(10),X(1000),Y(1000),Z(1000)
C     INPUT
      NS=1
      NI=1
      NF=1
      XS=0.0
      SI=0.0
      SF=0.0
      SSA=0.0
      SSX=0.0
      SIX=0.0
      READ(5,10)(SS(J),SI(J),SF(J),PA(J),PF(J),AV(J),
     * SSS(J),SII(J),SFF(J),J=1,10)
      READ(5,11)
   10 FORMAT(8F7.4,3F4.2,F5.2,2F3.0)
   11 FORMAT(F4.2)
C     SOURCE
      DO 40 I=1,1000
      X(I)=1.0
      Y(I)=0.0
      Z(I)=0.0
      CALL RLPSDT(1,V,A)
      E=1.6E-07
      WT=1.0
C     PATH LENGTH
   30 CALL SELECT(SS,SI,SF,PA,PF,AV,XS,XSS,XSI,XSF,A,E,RI,WT)
      XZERO=0.001
      EZERO=0.01
      IF(E.LT.EZERO.OR.WT.LT.ZEROWGT) GO
      CALL PATH(0,V,1,X(I),Y(I),Z(I),RI)
C     GEOMETRY
      RSQ=X(I)**2+Y(I)**2+Z(I)**2
      R=RSQ**2
      IF(RSQ.GT.RTOCT**2 GO
C     COLLISION
      CALL SCATTER(0,V,X,A,E)
      GOTO 30
```

PROGRAM ERROR Contd.

```
C     SECTI
   35 SP=1.0
      IF(I.GT.ESICOTO 36
      XSP=SP*AT
      I2=NP+1
      SS.3=SS.3+XSP**2
      GOTO 40
   36 SP=1.0E+03
      IF(I.GT.ESICOTO 37
      XSP=SP*AT
      I2=NP+1
      SSAI=SSAI+XSP**2
      GOTO 40
   37 XSP=SP*AT
      I2=NP+1
      SSAF=SSAF+XSP**2
   40 CONTINUE

C     OUTPUT

      STS=SQRT((SSAS/NS-(XSP/FLOAT(I2))**2)/NS)*3.09
      STI=SQRT((SSAI/NI-(XSP/FLOAT(I2))**2)/NI)*3.09
      STF=SQRT((SSAF/NF-(XSP/FLOAT(I2))**2)/NF)*3.09
      FACT=4.0E+11/(6.0*22.0/7.0)
      STS=FACT*STS/(100.0*SP)**2
      STI=FACT*STI/(100.0*SP)**2
      STF=FACT*STF/(100.0*SP)**2
      STS=STS*0.003
      STI=STI*0.003
      STF=STF*0.003
      SS=SQRT(SSAS*1.0E+11/(6.0*22.0/7.0))
      WRITE(6,2010)SP
   20 FORMAT(3X)'P=',3X,F4.2,2X,'SS=',E10.3,' ,E10.4)
      STOP
      END
```

APPENDIX D: OUTPUT OF COMPUTER PROGRAMS FOR 1000 NEUTRON HISTORIES

SHIELD RADIUS (M)	TRANSMISSION COEFF.	EQUIVALENT DOSE RATE (REM/HR)	EQUIVALENT DOSE RATE (REM/H	ERROR (REM/H
0.1	0.5[illegible]E+00	0.[illegible]E+05	0.[illegible]E+07	0.55E+05
0.2	0.8[illegible]E+00	0.[illegible]E+05	0.[illegible]E+05	0.16E+05
0.3	0.7[illegible]E+00	0.[illegible]E+04	0.[illegible]E+05	0.48E+04
0.4	0.4[illegible]E+00	0.[illegible]E+03	0.[illegible]E+05	0.15E+04
0.5	0.2[illegible]E+00	0.[illegible]E+03	0.[illegible]E+05	0.71E+03
0.6	0.[illegible]E+00	0.[illegible]E+03	0.[illegible]E+04	0.49E+03
0.7	0.[illegible]E+00	0.[illegible]E+03	0.[illegible]E+04	0.22E+03
0.8	0.[illegible]E+00	0.[illegible]E+03	0.[illegible]E+04	0.10E+03
0.9	0.[illegible]E-01	0.[illegible]E+02	0.[illegible]E+04	0.57E+02
1.0	0.[illegible]E-01	0.[illegible]E+02	0.[illegible]E+03	0.44E+02
1.1	0.[illegible]E-01	0.[illegible]E+02	0.[illegible]E+03	0.20E+02
1.2	0.[illegible]E-01	0.[illegible]E+01	0.[illegible]E+03	0.12E+02
1.3	0.[illegible]E-01	0.[illegible]E+01	0.[illegible]E+03	0.8[illegible]E+01
1.4	0.[illegible]E-01	0.[illegible]E+01	0.[illegible]E+03	0.30E+01
1.5	0.[illegible]E-01	0.[illegible]E+01	0.[illegible]E+02	0.22E+01
1.6	0.[illegible]E-01	0.[illegible]E+01	0.[illegible]E+02	0.17E+01
1.7	0.[illegible]E-01	0.[illegible]E+01	0.[illegible]E+02	0.15E+01
1.8	0.[illegible]E-02	0.[illegible]E+01	0.[illegible]E+02	0.10E+01
1.9	0.[illegible]E-02	0.[illegible]E+01	0.[illegible]E+02	0.10E+01
2.0	0.[illegible]E-02	0.[illegible]E+01	0.[illegible]E+01	0.54E+00
2.1	0.[illegible]E-02	0.[illegible]E+01	0.[illegible]E+01	0.43E+00
2.2	0.[illegible]E-02	0.[illegible]E+00	0.[illegible]E+01	0.30E+00
2.3	0.[illegible]E-03	0.[illegible]E+00	0.[illegible]E+01	0.18E+00
2.4	0.[illegible]E-03	0.[illegible]E+00	0.[illegible]E+01	0.14E+00
2.5	0.[illegible]E-03	0.[illegible]E+00	0.[illegible]E+00	0.11E+00

APPENDIX E: COMPOSITION OF ORDINARY CONCRETE AS DEFINED IN THIS PROJECT

Element	Atomic Mass (A.M.U.)	Density in Composition (g/cm^3)
Oxygen	16.00	1.1030
Silicon	28.06	0.2815
Aluminium	26.97	0.0330
Iron	55.85	0.0183
Calcium	40.08	0.7712
Carbon	12.01	0.0761
Sodium	23.00	0.0116
Potassium	39.10	0.0079
Hydrogen	01.01	0.0250
Magnesium	24.32	0.0426

(from Protection Against Neutron Radiation up to 30MeV. National Bureau of Standards Handbook 63, Nov. 1957, p. 81).

APPENDIX F: RANDOM NUMBERS

Random numbers are defined as sequence numbers which have equal chances of occuring. Random numbers are used in Monte Carlo computations, along with known nuclear data, to select the parameters which influence a particle's history. These include the direction of the first flight on leaving the source, the choice of interaction from those possible at each collision, the mean free path between collisions and the angle of emergence after collision.

It is therefore central to the application of Monte Carlo method that there should be readily available an adequate supply of random numbers. One method is to obtain pulses or counts from a truly random source, such as electrical noise or a radioactive substance. However it is more convenient to compute them by means of numerical algorithms specifically designed for this purpose.

Perhaps the most widely used random number generator is the multiplicative congruential method The algorithm is of the form

$$X_{n+1} = a\, X_n \pmod{m}$$

X_n; the starting value or 'seed', $x_n \geq 0$

a, the multiplier ; $a > 0$

m, the modulus, $m > X_n$, $m > a$

It is desirable that a sequence of random numbers should possess the following qualities:

(i) It should have a long period,

(ii) the numbers should be uniformly distributed, and

(iii) they should be independent.

In order to meet the qualities mentioned above, it recommended that (Profio, 1979):

(i) the number, m, be large, usually it is convenient to take it to be based on the computer's word size. That is for a binary machine of ρ bits, $m = 2^{\rho}$, and similarly for a decimal machine, $m = 10^{\rho}$.

(ii) the multiplier, a, should not be too small, or have a small number of one bits in its binary representation, or be close to a simple rational multiple of m or $\sqrt{m}$.

(iii) the initial random number, or seed be odd. It can be shown that sequences of this type have a period of $2^{\rho-2}$ if $m = 2^{\rho}$.