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METHODS OF BIASING SECONDARY GAMMA-RAY PRODUCTION IN COUPLED NEUTRON GAMMA-RAY MONTE CARLO CALCULATIONS+#

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ABSTRACT

Methods for applying importance sampling techniques to secondary gamma-ray generation in coupled, neutron-gamma-ray Monte Carlo transport calculations have been developed and evaluated. The Boltzmann transport equation is presented in an integral-matrix form which defines a set of coupled neutron-gamma-ray, multigroup equations and provides the basis for the coupled Monte Carlo random walk. Three methods of biasing the production of secondary gamma rays which make use of importance functions obtained from discrete ordinates adjoint calculations are formalized. These methods employ importance sampling techniques which include alteration of the gamma-ray generation probabilities, non-absorption weighting, and a combination of splitting and Russian roulette. These three methods are evaluated using the multigroup, Monte Carlo code MØRSE in the solution of a deep-penetration shielding problem in concrete. All three methods are shown to be more efficient than the standard method of biasing the secondary gamma-ray production in the MØRSE code. The methods varied from a factor of 1.3 to 40.0 better than the standard method based on the running time of the code and variance of the answer obtained.

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CHAPTER I

INTRODUCTION

The production of secondary gamma rays due to the interaction of neutrons within shielding materials creates a serious problem in the design of radiation shields. In deep-penetration transport problems their production and subsequent transport within a shield can contribute a major portion of the transmitted dose. For example, this is true of shields being optimized for weight in space applications, at large distances from the center of nuclear weapons bursts in air, or for thick shields used for reactor power plants.

Because of this importance of secondary gamma rays, the methods used to treat them in radiation transport calculations is a primary consideration in shield design. In the case of the Monte Carlo method of calculation these gamma rays must be incorporated into the random walk process in terms of the secondary gamma-ray production cross sections and corresponding energy spectra. Traditionally, this has been accomplished in separate Monte Carlo codes for the neutron and gamma-ray transport; however, more recently Monte Carlo codes have been written that employ "coupled" multigroup cross sections such that the combined neutron-gamma-ray problem may be solved simultaneously using a single code. However, the efficiency of running a combined problem, using either a single or separate code, can be largely dependent upon the techniques used in biasing the production of secondary gamma rays. This is especially true in the deep-penetration shielding problems where large numbers of secondary gamma rays may be produced which

never contribute to the answer. For example, in one approach that has been used gamma rays are generated at every neutron collision with the result that a large amount of computer time is spent in tracing unimportant gamma-ray histories. Obviously, importance sampling or biasing schemes are required to alter the gamma-ray production such that only important gamma rays are produced, i.e., the gamma rays which would have the best chance of contributing to the desired response.

Thus, the purpose of this work is to develop practical methods for and to demonstrate the calculational advantages of applying importance sampling techniques to secondary gamma-ray generation in coupled neutron-gamma-ray Monte Carlo transport calculations. Three basic methods have been developed and evaluated using the Monte Carlo code MORSE.[1] All of the methods make use of importance functions obtained from discrete ordinates adjoint calculations. These importance functions have been used to bias the secondary gamma-ray generation in energy and angle as well as in space.

In Chapter II, the coupled neutron-gamma-ray Boltzmann transport equation is presented in integral-matrix form which provides the basis for the coupled Monte Carlo random walk. The Monte Carlo method of obtaining the effect of interest is discussed along with an outline of the random walk process. The three methods of biasing the production of secondary gamma rays within the random walk process are then presented. These methods employ importance sampling techniques which include alteration of the gamma-ray generation probabilities, non-absorption weighting, and a combination of splitting and Russian roulette.

Chapter III presents the results of importance sampling the production of secondary gamma rays in deep-penetration shielding calculations using the multigroup Monte Carlo code MORSE. Results are given for a concrete shield for both a 14-MeV and a fission source. The three methods of importance sampling are compared based on the efficiency of obtaining an answer. This efficiency is considered to be proportional to the running time of the code and the variance of the answer obtained. The results of the Monte Carlo calculations are also compared with the results of the S_n code ANISN.[2]

Conclusions are discussed and recommendations are made in Chapter IV.

CHAPTER II

THEORY

The coupled neutron-gamma-ray transport equation and the formalization of the various techniques by which this coupling is obtained in Monte Carlo calculations are presented in this chapter. The coupled Boltzmann transport equation is presented in an integral-matrix form, defining a set of multigroup coupled neutron and gamma-ray equations. Methods of importance sampling the production of secondary gamma rays in the Monte Carlo random walk are developed in terms of these equations.

Coupled Neutron Gamma-Ray Boltzmann Transport Equation

The coupled Boltzmann transport equation can be written in the following integral-matrix form:

$$\chi(P) = S(P) + \int K(P \leftarrow P')\ \chi(P')dP' \quad , \qquad \text{(II-1)}$$

where the fundamental variable is the "emergent particle density" and $\chi(P)dP$* is the matrix of particles per unit time emerging in dP about P from a source or from real collisions, S(P)dP is the matrix of particles per unit time leaving a source in dP about P, and $K(P \leftarrow P')dP$ is the transition kernel matrix which is the matrix of particles per unit time emerging from collisions within dP about P given that a particle came out of collision at P'. The elements of these matrices

*Note that $P \equiv (\bar{r},\bar{\Omega})$ designates a point in position and direction space, and, thus, $\chi(P)$ is simply a way of indicating that the elements of this matrix are a function of space point $\bar{r}$, and direction $\bar{\Omega}$. This notation will be used hereafter to designate the functional dependence of the matrix elements.

**The word "particles" refers to both neutrons and gamma rays.

are first delineated according to the types of particle, i.e., either neutron or gamma ray:

$$\chi(P) = \begin{bmatrix} \chi^n(P) \\ \chi^\gamma(P) \end{bmatrix} \text{ emergent particle density matrix;}$$

$$S(P) = \begin{bmatrix} S^n(P) \\ S^\gamma(P) \end{bmatrix} \text{ source density matrix;}$$

$$K(P \leftarrow P') = C(P \leftarrow P')T(P \leftarrow P') \text{ transition kernel matrix,}$$

where

$$C(P \leftarrow P') = \begin{bmatrix} C^{nn}(P \leftarrow P') & C^{\gamma n}(P \leftarrow P') \\ C^{n\gamma}(P \leftarrow P') & C^{\gamma\gamma}(P \leftarrow P') \end{bmatrix} \text{ collision kernel matrix,}$$

$$T(P \leftarrow P') = \begin{bmatrix} T^n(P \leftarrow P') & 0 \\ 0 & T^\gamma(P \leftarrow P') \end{bmatrix} \text{transport kernel matrix.}$$

These elements are further delineated into N neutron energy groups and M minus N gamma-ray groups where M is the total number of energy groups:

$$\chi^n(P) = \begin{bmatrix} \chi_1^n(\bar{r},\bar{\Omega}) \\ \chi_2^n(\bar{r},\bar{\Omega}) \\ \vdots \\ \chi_N^n(\bar{r},\bar{\Omega}) \end{bmatrix}$$

where

$\chi_g^n(\bar{r},\bar{\Omega})d\bar{\Omega}$ = the number of neutrons per unit volume and time, emerging at space point $\bar{r}$ from a source or real

collision having energies within the gth energy group and directions which lie in $d\overline{\Omega}$ about $\overline{\Omega}$,

N = number of neutron groups.

$$\chi^{\gamma}(P) = \begin{bmatrix} \chi^{\gamma}_{N+1}(\overline{r},\overline{\Omega}) \\ \chi^{\gamma}_{N+2}(\overline{r},\overline{\Omega}) \\ \vdots \\ \chi^{\gamma}_{M}(\overline{r},\overline{\Omega}) \end{bmatrix}$$

where

$\chi^{\gamma}_{g}(\overline{r},\overline{\Omega})d\overline{\Omega}$ = the number of gamma rays per unit volume and time emerging at space point $\overline{r}$ from a source or real collision having energies within the gth group and directions which lie in $d\overline{\Omega}$ about $\overline{\Omega}$,

M = number of neutron groups plus the number of gamma-ray groups.

$$S^{n}(P) = \begin{bmatrix} S^{n}_{1}(\overline{r},\overline{\Omega}) \\ S^{n}_{2}(\overline{r},\overline{\Omega}) \\ \vdots \\ S^{n}_{N}(\overline{r},\overline{\Omega}) \end{bmatrix}$$

where

$S^{n}_{g}(r,\overline{\Omega})d\overline{\Omega}$ = source neutrons emitted per unit volume and time at space point $\overline{r}$ having energies within group g and directions which lie in $d\overline{\Omega}$ about $\overline{\Omega}$.

$$S^{\gamma}(P) = \begin{bmatrix} S^{\gamma}_{N+1}(\bar{r},\bar{\Omega}) \\ S^{\gamma}_{N+2}(\bar{r},\bar{\Omega}) \\ \vdots \\ S^{\gamma}_{M}(\bar{r},\bar{\Omega}) \end{bmatrix}$$

where

$S^{\gamma}_{g}(r,\bar{\Omega})d\bar{\Omega}$ = source gamma rays emitted per unit volume and time at space point $\bar{r}$, having energies within group g and directions which lie in $d\bar{\Omega}$ about $\bar{\Omega}$.

Neutron Collision Matrix

$$C^{nn}(P \leftarrow P') = \begin{bmatrix} C^{nn}_{1\leftarrow 1} & C^{nn}_{1\leftarrow 2} & \cdots & C^{nn}_{1\leftarrow N} \\ C^{nn}_{2\leftarrow 1} & C^{nn}_{2\leftarrow 2} & \cdots & C^{nn}_{2\leftarrow N} \\ \vdots & \vdots & & \vdots \\ C^{nn}_{N\leftarrow 1} & C^{nn}_{N\leftarrow 2} & \cdots & C^{nn}_{N\leftarrow N} \end{bmatrix}$$

where

$$C^{nn}_{g\leftarrow g'} = C^{nn}_{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') = \frac{\Sigma^{g\leftarrow g'}_{s_n}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma^{g'}_{s_n}(\bar{r})} \times \frac{\Sigma^{g'}_{s_n}(\bar{r})}{\Sigma^{g'}_{t_n}(\bar{r})}$$

$\dfrac{\Sigma^{g\leftarrow g'}_{s_n}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')d\bar{\Omega}}{\Sigma^{g'}_{s_n}(\bar{r})}$ = normalized probability density function; the probability that a neutron in energy group g' and with an initial direction Ω'' undergoes a collision at $\bar{r}$ which places it into a new energy group g, and a direction that lies in $d\bar{\Omega}$ about $\bar{\Omega}$,

$$\frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})}$$ = average number of neutrons* emerging from a collision at $\bar{r}$ given that a neutron in energy group g' has a collision at $\bar{r}$,

$\Sigma_{s_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')$ = neutron to neutron energy-averaged transfer cross section** which includes all neutron producing reactions,

$\Sigma_{t_n}^{g'}(\bar{r})$ = energy-averaged neutron total cross section for the g'th group,

$\Sigma_{s_n}^{g'}(\bar{r})$ = energy-averaged neutron production cross section for the g'th group

$$= \sum_{g=1}^{N} \int d\bar{\Omega}\ \Sigma_{s_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')$$

Secondary Gamma-Ray Generation Matrix

$$C^{n\gamma}(P\leftarrow P') = \begin{bmatrix} C_{N+1\leftarrow 1}^{n\gamma} & C_{N+1\leftarrow 2}^{n\gamma} & \cdots & C_{N+1\leftarrow N}^{n\gamma} \\ C_{N+2\leftarrow 1}^{n\gamma} & C_{N+2\leftarrow 1}^{n\gamma} & \cdots & C_{N+2\leftarrow N}^{n\gamma} \\ \vdots & \vdots & & \vdots \\ C_{M\leftarrow 1}^{n\gamma} & C_{M\leftarrow 2}^{n\gamma} & \cdots & C_{M\leftarrow N}^{n\gamma} \end{bmatrix}$$

where

$$C_{g\leftarrow g'}^{n\gamma} = C_{g\leftarrow g'}^{n\gamma}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') = \frac{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{c_n}^{g'}(\bar{r})} \times \frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})}$$

---

*Note that for reactions such as (n,2n) more than one neutron may emerge from the collision.

**Definitions of all flux-weighted, energy-averaged cross sections used throughout this thesis are given in Appendix A.

$$\frac{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')d\bar{\Omega}}{\Sigma_{c_n}^{g'}(\bar{r})}$$ = normalized probability density function; the probability that a neutron in energy group g' and with an initial direction $\bar{\Omega}''$ undergoes an event at $\bar{r}$ which produces a gamma ray into energy group g and a direction which lies in $d\bar{\Omega}$ about $\bar{\Omega}$,

$$\frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})}$$ = average number of gamma rays emerging from a collision at $\bar{r}$ given that a neutron in energy group g' has a collision at $\bar{r}$,

$\Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')$ = neutron to gamma-ray energy-averaged transfer cross section which includes all neutron reactions from which a gamma ray results.

$\Sigma_{c_n}^{g'}(\bar{r})$ = energy-averaged, neutron-to-gamma-ray production cross section for the g'<u>th</u> group,

$$= \sum_{g=1}^{N} \int d\bar{\Omega}\ \Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') \ .$$

<u>Gamma-Ray Collision Matrix</u>

$$C^{\gamma\gamma}(P\leftarrow P') = \begin{bmatrix} C^{\gamma\gamma}_{N+1\leftarrow N+1} & C^{\gamma\gamma}_{N+1\leftarrow N+2} & \cdots & C^{\gamma\gamma}_{N+1\leftarrow M} \\ C^{\gamma\gamma}_{N+2\leftarrow N+1} & C^{\gamma\gamma}_{N+2\leftarrow N+2} & \cdots & C^{\gamma\gamma}_{N+2\leftarrow M} \\ \vdots & \vdots & & \vdots \\ C^{\gamma\gamma}_{M\leftarrow N+1} & C^{\gamma\gamma}_{M\leftarrow N+2} & \cdots & C^{\gamma\gamma}_{M\leftarrow M} \end{bmatrix}$$

where

$$C^{\gamma\gamma}_{g\leftarrow g} = C^{\gamma\gamma}_{g\leftarrow g}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') = \frac{\Sigma_{s_\gamma}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{s_\gamma}^{g'}(\bar{r})} \times \frac{\Sigma_{s_\gamma}^{g'}(\bar{r})}{\Sigma_{t_\gamma}^{g'}(\bar{r})}$$

$$\frac{\Sigma_{s_\gamma}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')\,d\bar{\Omega}}{\Sigma_{s_\gamma}^{g'}(\bar{r})}$$ = normalized probability density function; the probability that a gamma ray in energy group g' and with an initial direction $\bar{\Omega}''$ undergoes an event at $\bar{r}$ which places it into energy group g and a direction which lies in $d\bar{\Omega}$ about $\bar{\Omega}$,

$$\frac{\Sigma_{s_\gamma}^{g'}(\bar{r})}{\Sigma_{t_\gamma}^{g'}(\bar{r})}$$ = average number of gamma rays* emerging from a collision at $\bar{r}$ given that a gamma ray in energy group g' has a collision at $\bar{r}$,

$\Sigma_{s_\gamma}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')$ = gamma ray to gamma ray energy-averaged transfer cross section which includes Compton scattering and pair production,

$\Sigma_{t_\gamma}^{g'}(\bar{r})$ = energy-averaged gamma-ray total cross section for the g'th group,

$\Sigma_{s_\gamma}^{g'}(\bar{r})$ = energy-averaged gamma-ray production cross section for the g'th group,

$$= \sum_{g=N+1}^{M} \int d\bar{\Omega}\; \Sigma_{s_\gamma}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') \quad .$$

Photoneutron Production Matrix

$$C^{\gamma n}(P\leftarrow P') = \begin{bmatrix} C_{1\leftarrow N+1}^{\gamma n} & C_{1\leftarrow N+2}^{\gamma n} & \cdots & C_{1\leftarrow M}^{\gamma n} \\ C_{2\leftarrow N+1}^{\gamma n} & C_{2\leftarrow N+2}^{\gamma n} & \cdots & C_{2\leftarrow M}^{\gamma n} \\ \vdots & \vdots & & \vdots \\ C_{N\leftarrow N+1}^{\gamma n} & C_{N\leftarrow N+2}^{\gamma n} & \cdots & C_{N\leftarrow M}^{\gamma n} \end{bmatrix}$$

*Note that a pair production reaction is assumed to result in two gamma rays emerging from a collision.

where

$$C^{\gamma n}_{g\leftarrow g'} = C^{\gamma n}_{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') = \frac{\Sigma^{g\leftarrow g'}_{c_\gamma}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma^{g'}_{c_\gamma}(\bar{r})} \times \frac{\Sigma^{g'}_{c_\gamma}(\bar{r})}{\Sigma^{g'}_{t_\gamma}(\bar{r})}$$

$\dfrac{\Sigma^{g\leftarrow g'}_{c_\gamma}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')\,d\bar{\Omega}}{\Sigma^{g'}_{c_\gamma}(\bar{r})}$ = normalized probability density function; the probability that a gamma ray in energy group g' and with an initial direction $\bar{\Omega}''$ undergoes a collision at $\bar{r}$ which produces a neutron at $\bar{r}$ in energy group g and a direction which lies in $d\bar{\Omega}$ about $\bar{\Omega}$,

$\dfrac{\Sigma^{g'}_{c_\gamma}(\bar{r})}{\Sigma^{g'}_{t_\gamma}(\bar{r})}$ = average number of neutrons emerging from a collision at $\bar{r}$ given that a gamma ray in energy group g' has a collision at $\bar{r}$,

$\Sigma^{g\leftarrow g'}_{c_\gamma}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')$ = gamma ray to neutron energy-averaged transfer cross section which includes photoneutron production,

$\Sigma^{g'}_{c_\gamma}(\bar{r})$ = energy-averaged, gamma-ray-to-neutron production cross section for the g'<u>th</u> group,

$$= \sum_{g=N+1}^{M} \int d\bar{\Omega}\, \Sigma^{g\leftarrow g'}_{c_\gamma}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') \quad .$$

<u>Neutron Transport Matrix (Diagonal Matrix)</u>

$$T^n(P\leftarrow P') = \begin{bmatrix} T^n_1 & 0 & \dots & 0 \\ 0 & T^n_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & T^n_N \end{bmatrix}$$

where

$$T_g^n = T_g^n(\bar{r}\leftarrow\bar{r}',\bar{\Omega}') = \Sigma_{t_n}^g(\bar{r})\, e^{-\int_0^R \Sigma_{t_n}^g(\bar{r}-R'\bar{\Omega}')dR'} \frac{\delta(\bar{\Omega}',\bar{\Omega}'')}{R^2}$$

$$\Sigma_{t_n}^g(\bar{r})\, e^{-\int_0^R \Sigma_{t_n}^g(\bar{r}-R'\bar{\Omega}'')dR'} dR$$

= probability that a neutron which emerges from a collision at $\bar{r}'$ with coordinates (group g, $\bar{\Omega}''$) will experience an event in dR about $\bar{r} = \bar{r}' + R\bar{\Omega}''$.

<u>Gamma-Ray Transport Matrix (Diagonal Matrix)</u>

$$T^\gamma(P\leftarrow P') = \begin{bmatrix} T_{N+1}^\gamma & 0 & \cdots & 0 \\ 0 & T_{N+2}^\gamma & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & T_M^\gamma \end{bmatrix}$$

where

$$T_g^\gamma = T_g^\gamma(\bar{r}\leftarrow\bar{r}',\bar{\Omega}') = \Sigma_{t_\gamma}^g(\bar{r})e^{-\int_0^R \Sigma_{t_\gamma}^g(\bar{r}-R'\bar{\Omega}')\, dR'} \frac{\delta(\bar{\Omega}',\bar{\Omega}'')}{R^2}$$

$$\Sigma_{t_\gamma}^g(\bar{r})\, e^{-\int_0^R \Sigma_{t_\gamma}^g(\bar{r}-\bar{R}'\bar{\Omega}'')dR'} dR$$

= probability that a gamma ray which emerges from a collision at $\bar{r}'$ with coordinates (group g, $\bar{\Omega}''$) will experience an event in dR about $\bar{r} = \bar{r}' + R\bar{\Omega}''$.

The delta function must appear in the transport kernel since only those particles emerging from collisions at $\bar{r}'$ which are directed along the positive $\bar{\Omega}''$ direction can contribute at $\bar{r}$ (see Appendix A). The delta function has the property that for any function $f(\bar{\Omega}')$,

$$\int^{\Omega'} f(\bar{\Omega}')\ \delta(\bar{\Omega}',\bar{\Omega}'')d\bar{\Omega}' = f(\bar{\Omega}'')$$

where the angles $\bar{\Omega}''$ and $\bar{\Omega}'$ are specified in Figure II-1.

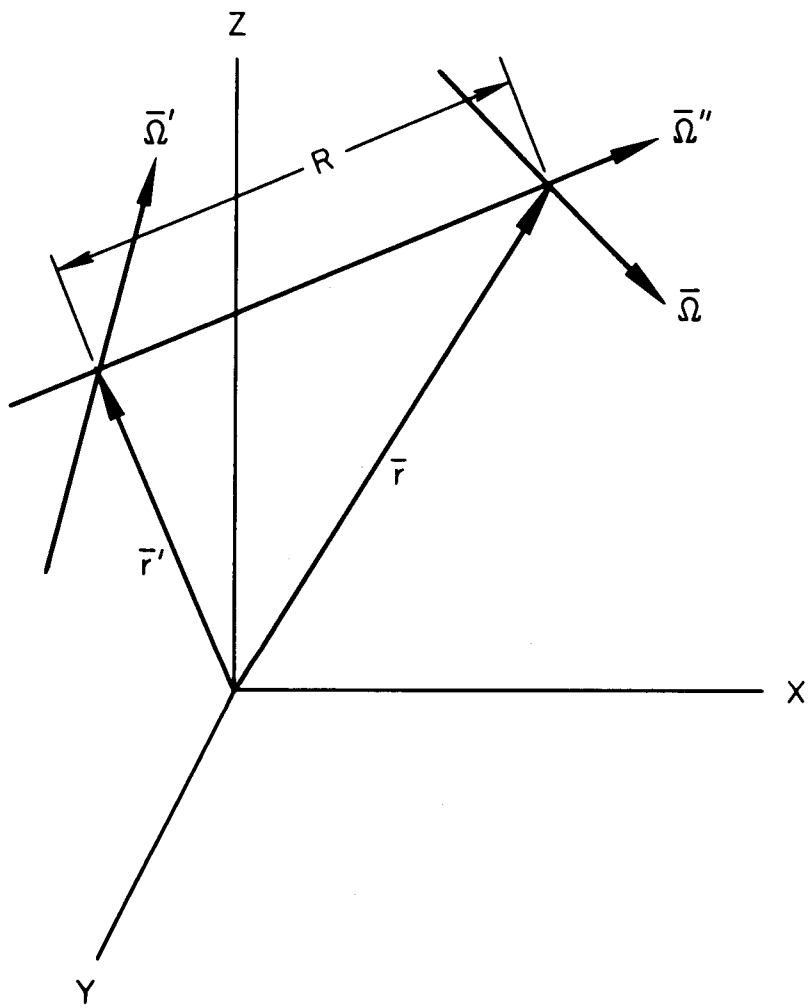

Figure II-1: Coordinate System for Equations II-2 and II-3.

R = spatial variable which relates a fixed point in space ($\bar{r}$) to an arbitrary point ($\bar{r}'$).

$\bar{\Omega}'$ = the direction of particles emerging from collisions at $\bar{r}'$.

$\bar{\Omega}''$ = the required direction for particles traveling from $\bar{r}'$ to $\bar{r}$.

$\bar{\Omega}$ = the direction of particles emerging from collision at $\bar{r}$.

$\bar{r}' = \bar{r} - R\bar{\Omega}''$.

$dP = d\bar{\Omega}d\bar{r}$.

$dP' = d\bar{\Omega}''d\bar{r}'$.

With these definitions, the matrix equation (Eq. II-1) represents a set of multigroup equations which are coupled through the collision kernel matrix $C(P \leftarrow P')$. General assumptions are now made regarding the form of $C(P \leftarrow P')$ which alter this set of equations. Although these assumptions are not essential, they are made at this point for simplicity. The assumptions, along with the corresponding changes in $C(P \leftarrow P')$ are as follows:

1. photoneutron production is assumed to be zero which implies $C^{\gamma n}(P \leftarrow P')$ is a zero matrix,
2. neutron upscatter (neutron transfer from a lower to higher neutron energy group) is assumed to be zero which implies that $C^{nn}(P \leftarrow P')$ is a lower diagonal matrix (all elements above the diagonal are zero), and
3. gamma-ray upscatter (gamma-ray transfer from a lower to higher gamma-ray energy group) is assumed to be zero which implies that $C^{\gamma\gamma}(P \leftarrow P')$ is a lower diagonal matrix.

With these assumptions regarding the collision kernel it is instructive to examine the individual group equations represented by

Eq. (II-1). First consider the typical neutron equation* for group g, $1 \leq g \leq N$:

$$\chi_g^n(\bar{r},\bar{\Omega}) = S_g^n(\bar{r},\bar{\Omega}) \tag{II-2}$$

$$+ \sum_{g'=g}^{1} \int^{\bar{r}'} \int^{4\pi} C_{g\leftarrow g'}^{nn}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') \; T_{g'}^{n}(\bar{r}\leftarrow\bar{r}',\bar{\Omega}') \; \chi_{g'}^{n}(\bar{r}',\bar{\Omega}')d\bar{\Omega}''d\bar{r}'$$

Thus the contributions to $\chi_g^n(\bar{r},\bar{\Omega})$ are made up of direct source contributions from neutron group g plus inscattering contributions from group g and all neutron groups g' of higher energy.

Now consider the typical gamma-ray equation for group g, $N + 1 \leq g \leq M$:

$$\chi_g^\gamma(\bar{r},\bar{\Omega}) = S_g^\gamma(\bar{r},\bar{\Omega}) \tag{II-3}$$

$$+ \sum_{g'=g}^{N+1} \int^{\bar{r}'} \int^{4\pi} C_{g\leftarrow g'}^{\gamma\gamma}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') \; T_{g'}^{\gamma}(\bar{r}\leftarrow\bar{r}',\bar{\Omega}') \; \chi_{g'}^{\gamma}(\bar{r}',\bar{\Omega}')d\bar{\Omega}''d\bar{r}'$$

$$+ \sum_{g'=N}^{1} \int^{\bar{r}'} \int^{4\pi} C_{g\leftarrow g'}^{n\gamma}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'') \; T_{g'}^{n}(\bar{r}\leftarrow\bar{r}',\bar{\Omega}') \; \chi_{g'}^{n}(\bar{r}',\bar{\Omega}')d\bar{\Omega}''d\bar{r}' \; .$$

Thus, the contributions to $\chi_g^\gamma(\bar{r},\bar{\Omega})$ are made up of direct source contributions from gamma-ray group g plus inscattering from group g and all gamma-ray groups g' of higher energy and from neutron collision events (which produce gamma rays) in all neutron groups.

An assumption is also made regarding the angular dependence of the previously defined cross sections. These cross sections have been

*See Appendix A for derivation of this group equation from the integro-differential form of the Boltzmann transport equation.

shown to be a function of $\overline{\Omega}''$ and $\overline{\Omega}$; however, it is assumed that they are independent of the incoming particle direction Ω'' and only a function of $\overline{\Omega}''\cdot\overline{\Omega}$, i.e., the cosine of the angle between $\overline{\Omega}''$ and $\overline{\Omega}$.

Effect of Interest

The solutions usually being sought in radiation transport problems is some particular quantity like the total dose at the outside surface of a shield or the heating rate in the control rods of a reactor. This solution is referred to as the "effect of interest" and denoted λ. The effect of interest λ can be expressed in terms of the emergent particle density by

$$\lambda = \int R(P)\ \chi(P)dP \qquad \text{(II-4)}$$

where R(P) is a row-matrix response function

$$R(P) = [R_1(\overline{r},\overline{\Omega}),\quad R_2(\overline{r},\overline{\Omega})\quad \ldots\quad R_M(\overline{r},\overline{\Omega})]$$

where

$R_g(\overline{r},\overline{\Omega})$ = the response function of the effect of interest due to a neutron which emerges from a collision having phase space coordinates (group g, $\overline{r},\overline{\Omega}$), $1 \leq g \leq N$,

$R_g(\overline{r},\overline{\Omega})$ = the response function of the effect of interest due to a gamma ray which emerges from a collision having phase space coordinates (group g, $\overline{r},\overline{\Omega}$), $N+1 \leq g \leq M$.

The Monte Carlo Procedure

The Monte Carlo procedure for obtaining an estimate of the effect of interest λ consists of two basic steps. First, the random walk process is used to sample the distribution of neutrons and gamma rays as defined by equation (II-1). Large numbers of particle histories are generated which are random samples from the emergent particle density p.d.f. $X(P)$. This collection of particle event descriptions can be denoted by

$$(\bar{r}_{0_j}, g_{0_j}, \bar{\Omega}_{0_j})\ (\bar{r}_{1_j}, g_{1_j}, \bar{\Omega}_{1_j})\ \ldots\ (\bar{r}_{D_j}, g_{D_j}, \bar{\Omega}_{D_j})$$

where D_j is the number of collisions for a given history j. Secondarily, an estimate of λ, $\hat{\lambda}$, is computed as

$$\hat{\lambda} = \frac{1}{J} \sum_{j=1}^{J} \sum_{g=1}^{M} \sum_{d=0}^{D_j} R_{g_{d_j}} (\bar{r}_{d_j}, \bar{\Omega}_{d_j}) \qquad \text{(II-5)}$$

where

D_j = number of collisions for j<u>th</u> history,

d = collision number for the j<u>th</u> history,

J = total number of histories,

$R_{g_{d_j}} (\bar{r}_{d_j}, \bar{\Omega}_{d_j})$ = response function evaluated at the phase space coordinates of the d<u>th</u> collision for the j<u>th</u> history.

If J is large enough (i.e., if a sufficient number of particle histories are sampled) then the value of $\hat{\lambda}$ will approach the expected value λ.[3]

Importance Sampling

Importance sampling involves a distortion of the actual physical transition probabilities such that events of interest in the calculation will occur more frequently than in the analog process. (Events of interest are those events which contribute, directly or potentially, most heavily to the desired answer.) This may involve the alteration of the source term S(P) or the transition kernel $K(P \leftarrow P')$ or both, and the subsequent generation of particle histories from these altered probability density functions in the Monte Carlo random walk. However, if the estimate of the effect of interest is not to be affected, this biasing must be compensated for in some way. This may be accomplished in the random walk process by adjusting the statistical weight associated with each of the particle histories. In the analog random walk the weight of the particle would remain equal to its initial value as the particle moves from site to site. However, in the biased random walk where the particle histories are constructed from these altered distributions, this weight must be adjusted at each transition by the ratio of the natural distribution to the biased distribution.

With this procedure the estimate of λ is given by[4]

$$\hat{\lambda} = \frac{1}{J} \sum_{j=1}^{J} \sum_{g=1}^{M} \sum_{d=0}^{D_j} R_{g_{d_j}} (\bar{r}_{d_j}, \bar{\Omega}_{d_j}) \, W_g(\bar{r}_{d_j}) \qquad \text{(II-6)}$$

where $W_g(\bar{r}_{d_j})$ is the weight of the j<u>th</u> particle leaving the d<u>th</u> collision.

Generally the application of importance sampling involves the use of a function I(P) to modify the source S(P) and/or the transition

kernel $K(P \leftarrow P')$ where $I(P)$ is referred to as an importance function and is a measure of the importance (to the effect of interest) of particles emerging from collisions at P. Ideally the application of a proper importance function would result in a very small variance of the mean. Coveyou *et al.* have shown a very good choice of this importance function to be the adjoint flux $J(P)$ which is the solution to the adjoint of equation (II-1), and is defined as the expected contribution to the answer that these particles will yield leaving the present and all subsequent collisions until they are absorbed or leave the configuration.[5] Therefore $J(P)$ or a function which is similar to $J(P)$ is normally a reasonable choice for an importance function.

Analog Secondary Gamma-Ray Generation

In order to describe secondary gamma-ray generation as an analog of the physical process, it would be necessary to have the total neutron cross section in terms of the individual neutron reaction types along with the multiplicity of neutrons and gamma rays produced and corresponding energy spectra. Then the probability of a particular reaction type occurring is given by the ratio of the cross section for that reaction to the total neutron cross section and the number of gamma rays produced is given by the corresponding multiplicity for that particular reaction. However, in multigroup cross section format all neutron reactions which produce neutrons are included in the neutron-to-neutron transfer cross sections and all neutron reactions which produce gamma rays are included in the neutron-to-gamma-ray transfer cross sections as previously defined. Therefore, the coupled Boltzmann transport equation in multi-

group form has been written such that the specific reaction types do not appear independently. Consequently the Monte Carlo simulation of neutron and gamma-ray transport according to this equation cannot be an analog process and appropriate weight adjustments must be applied to particle histories so generated. In order to determine what these adjustments should be, it is necessary to consider what the average weight of particles leaving a neutron collision would be in the analog case. To do this, the individual neutron reaction cross sections and corresponding average multiplicity of neutron and gamma rays are assumed to be known and defined as follows:

Σ_i = neutron reaction cross section for the ith reaction type,

Σ_t = total neutron cross section,

$= \sum_{i=1}^{Q} \Sigma_i$

k_{i_n} = average number of neutrons produced for the ith type reaction,

k_{i_γ} = average number of gamma rays produced for the ith type reaction, and

Q = total number of reaction types.

With these definitions the average weight, <W>, leaving a neutron collision due to an incoming neutron of weight W' is given by

$$\langle W \rangle = W' \times \sum_{i=1}^{Q} k_{i_n} \frac{\Sigma_i}{\Sigma_t} + W' \times \sum_{i=1}^{Q} k_{i_\gamma} \frac{\Sigma_i}{\Sigma_t} \qquad \text{(II-7)}$$

where the two summations represent the average number of neutrons and gamma rays produced multiplied by the respective probability for their production and summed over all possible reactions.

The first term on the right hand side of equation (II-7) is the average weight of neutrons leaving the collision and the second term is the average weight of gamma rays leaving the collision. For a given neutron group g' and space point $\bar{r}$, this equation may be expressed in terms of the multigroup cross sections previously defined:

$$\langle W(\bar{r})\rangle = W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} + W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \quad . \tag{II-8}$$

This equation then gives the average weight* of particles leaving a collision at $\bar{r}$ due to a neutron collision in group g' at $\bar{r}$ in the analog case. Similarly it can be shown that the average weight leaving a gamma-ray collision in the absence of photoneutron production is given by

$$\langle W(\bar{r})\rangle = W_{g'}(\bar{r}) \times \frac{\Sigma_{s_\gamma}^{g'}(\bar{r})}{\Sigma_{t_\gamma}^{g'}(\bar{r})} \quad . \tag{II-9}$$

It would not be practical to use analog Monte Carlo in the production of secondary gamma rays not only because of the additional detail in the cross-section data that would be required, but also the computations would be grossly inefficient. For example, in deep-penetration shielding problems analog sampling may not within a reasonable period of time yield any gamma-ray histories traveling through the regions of interest. Even when a few histories that make important contributions are obtained, the probable error may be very large, and increasing the number of histories decreases the error only slowly (inversely to the square root of the number of histories). Then, just as in other aspects of Monte Carlo, the application of importance sampling techniques to

*The weight with no group subscript indicates the outgoing group has not yet been specified.

the production of secondary gamma rays is essential in deep-penetration shielding problems. However, in any importance sampling scheme which is applied to the collision process, the average weight of particles leaving a neutron or gamma-ray collision must be maintained at the average value given by the previous equations or else a bias is introduced.

The Random Walk in the Coupled Multigroup Monte Carlo Calculation

An outline of a procedure for generating a sequence of particle histories by the random walk process from the probability distribution functions S(P) and K(P←P') defined in equation (II-1) is as follows:

Step 1. Source

An initial particle position, energy and angle are chosen and weight $W_g(\bar{r})$ assigned from the probability density function S(P). Choose g_o, $\bar{r}_o$, and $\bar{\Omega}_o$ from

$$\frac{S(P)}{\sum_{g=1}^{M} \iint S_g(\bar{r},\bar{\Omega})\,d\bar{r}\,d\bar{\Omega}} \quad .$$

Set weight

$$W_{g_o}(\bar{r}_o) = \sum_{g=1}^{M} \iint S_g(\bar{r},\bar{\Omega})\,d\bar{r}\,d\bar{\Omega} \quad .$$

In some cases the source distribution is a properly normalized p.d.f. and each source particle has an initial weight of unity. During the random walk $W_g(\bar{r})$ will denote the expected weight density of particles leaving collisions at $\bar{r}$ in group g.

Step 2. Transport

The particle is transported to the next collision site, $\bar{r}_1$, according to the transport probability density function. Select a flight path R from

$$\Sigma_{t_n}^{g_o}(\bar{r}_1)\, e^{-\int_o^R \Sigma_{t_n}^{g_o}(\bar{r}_1 - R'\bar{\Omega}_o)dR'} \qquad \text{if } 1 \le g_o \le N \quad ,$$

$$\Sigma_{t_\gamma}^{g_o}(\bar{r}_1)\, e^{-\int_o^R \Sigma_{t_\gamma}^{g_o}(\bar{r}_1 - R'\bar{\Omega}_o)dR'} \qquad \text{if } N+1 \le g_o \le M$$

and set $\bar{r}_1 = \bar{r}_0 + R\bar{\Omega}_0$. If $\bar{r}_1$ is outside the system of interest the particle has escaped and the history is terminated.

Step 3. Collision

Require that the particle survive the collision by adjusting the weight for nonabsorption according to

$$W(\bar{r}_1) = W_{g_o}(\bar{r}_o) \times \frac{\Sigma_{s_n}^{g_o}(\bar{r}_1)}{\Sigma_{t_n}^{g_o}(\bar{r}_1)} \qquad \text{if } 1 \le g_o \le N \text{ (i.e., the particle is a neutron)},$$

or according to

$$W(\bar{r}_1) = W_{g_o}(\bar{r}_o) \times \frac{\Sigma_{s_\gamma}^{g_o}(\bar{r}_1)}{\Sigma_{t_\gamma}^{g_o}(\bar{r}_1)} \qquad \text{if } N+1 \le g_o \le M \text{ (i.e., the particle is a gamma ray)}.$$

If $1 \leq g_o \leq N$, require a secondary gamma ray to be produced with the weight given by

$$W(\bar{r}_1) = W_{g_o}(\bar{r}_o) \times \frac{\Sigma_{c_n}^{g_o}(\bar{r}_1)}{\Sigma_{t_n}^{g_o}(\bar{r}_1)} \quad .$$

In each of the above cases the weight is adjusted to the average value of the analog case given by equations (II-8) and (II-9). (Note that the weight with no group subscript indicates that the outgoing group has not yet been selected.)

Step 4. Selection of Exit Energy Group and Angle

If $1 \leq g_o \leq N$, select a new neutron group g_1 according to the p.d.f.

$$\frac{\int d\bar{\Omega}\ \Sigma_{s_n}^{g \leftarrow g_o}(\bar{r}_1, \bar{\Omega} \leftarrow \bar{\Omega}_o)}{\Sigma_{s_n}^{g_o}(\bar{r}_1)} \qquad g = (g_o, g_o+1, \ldots N)$$

and select a new neutron direction $\bar{\Omega}$ from

$$\frac{\Sigma_{s_n}^{g_1 \leftarrow g_o}(\bar{r}_1, \bar{\Omega} \leftarrow \bar{\Omega}_o)}{\Sigma_{s_n}^{g_1 \leftarrow g_o}(\bar{r}_1)} \quad .$$

Select a gamma-ray group g_2 according to the p.d.f.

$$\frac{\int d\bar{\Omega}\ \Sigma_{c_n}^{g \leftarrow g_o}(\bar{r}, \bar{\Omega} \leftarrow \bar{\Omega}_o)}{\Sigma_{c_n}^{g_o}(\bar{r}_1)} \qquad g = (N+1, N+2 \ldots M)$$

and a new gamma-ray direction from

$$\frac{\Sigma_{c_n}^{g_2 \leftarrow g_o}(\bar{r}_1, \bar{\Omega} \leftarrow \bar{\Omega}_o)}{\Sigma_{c_n}^{g_2 \leftarrow g_o}(\bar{r}_1)} \quad .$$

If $N+1 \leq g_o \leq M$, select a new gamma-ray group g_1 according to the p.d.f.

$$\frac{\int d\Omega \; \Sigma_{s_\gamma}^{g \leftarrow g_o}(\bar{r}_1, \bar{\Omega} \leftarrow \bar{\Omega}_o)}{\Sigma_{s_\gamma}^{g_o}(\bar{r}_1)} \qquad g = (g_o, g_o+1, \ldots M)$$

and a new direction $\bar{\Omega}$ from

$$\frac{\Sigma_{s_\gamma}^{g_1 \leftarrow g_o}(\bar{r}_1, \bar{\Omega} \leftarrow \bar{\Omega}_o)}{\Sigma_{s_\gamma}^{g_1 \leftarrow g_o}(\bar{r}_1)} \quad .$$

If the new energy groups of the particles is below the energy range of interest the history is terminated and this procedure begins again at step 1. If the history is not terminated the procedure returns to step 2.

The secondary gamma ray's source position $\bar{r}_1$, group g_2, angle of emission $\bar{\Omega}$ and weight $W_{g_2}(\bar{r}_1)$ are stored for future processing through steps 2 through 4.

Importance Sampling the Production of Secondary Gamma Rays

Method I: Combined Problem as a Single-Type Particle Problem with Nonabsorption Weighting

In the analog random walk a neutron collision survival test is performed at every neutron collision to decide whether the neutron emerges or not. The survival probability for a neutron in group g' at $\bar{r}$ is given by the nonabsorption probability which is the previously defined cross-section ratio $\Sigma_{s_n}^{g'}(\bar{r})/\Sigma_{t_n}^{g'}(\bar{r})$ excluding the multiplicity factor. The neutron statistical weight remains unchanged if it survives the collision and is set equal to zero if it is absorbed. However, if nonabsorption weighting is used as a means of importance sampling, instead of determining the probability of absorption or survival, the particle is forced to survive and a weight modification is introduced to account for this biased sampling. Thus if the incoming weight is $W_{g'}(\bar{r})$, the emerging weight is

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \tag{II-10}$$

where the multiplicity of neutrons included as part of the nonabsorption probability accounts for more than one neutron being produced in the collision process. This type of importance sampling, generally referred to as "survival biasing," changes only the survival probability without essential change in the collision kernel.

One method of allowing for importance sampling the production of secondary gamma rays, which is analogous to survival biasing, is to treat the coupled transport problem as a single-type particle transport such that the result of any collision is always a single particle. A

nonabsorption weight adjustment is then made to account for this biased particle production.

With this method the production of secondary gamma rays is simply a consequence of selecting a transfer to group g where $N+1 \leq g \leq M$ without any reference to the type of particle being transferred. (Distinction between neutron and gamma rays is allowed for in the analysis portion of the Monte Carlo code in order that individual responses can be calculated.)

In this case the survival probability of a particle at each collision is certainty, and the corresponding nonabsorption weight correction for an incoming particle of weight $W_{g'}(\bar{r})$ in group g' is given by

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r}) + \Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \tag{II-11}$$

for $1 \leq g' \leq N$ and

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{s_\gamma}^{g'}(\bar{r})}{\Sigma_{t_\gamma}^{g'}(\bar{r})} \tag{II-12}$$

for $N+1 \leq g' \leq M$.

With this procedure the average weight leaving the collision is the same as in the analog case [equations (II-8) and (II-9)]; however, this weight is carried by a single particle.

The proper distribution of this weight between the neutron and gamma-ray groups is allowed for by selecting an outgoing group g for this particle according to the normalized p.d.f. $P^{g \leftarrow g}(\bar{r})$ which is the set of discrete group-to-group transfer probabilities given by

$$P^{g\leftarrow g'}(\bar{r}) = \begin{cases} \dfrac{\int d\bar{\Omega}\ \Sigma_{s_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{s_n}^{g'}(\bar{r}) + \Sigma_{c_n}^{g'}(\bar{r})}, & g = (g',g'+1\ldots N) \\[2ex] \dfrac{\int d\bar{\Omega}\ \Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{s_n}^{g'}(\bar{r}) + \Sigma_{c_n}^{g'}(\bar{r})}, & g = (N+1,N+2\ldots M) \end{cases} \qquad \text{(II-13)}$$

for $1 \leq g' \leq N$.

$$P^{g\leftarrow g'}(\bar{r}) = \frac{\int d\bar{\Omega}\ \Sigma_{s_\gamma}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{s_\gamma}^{g'}(\bar{r})}, \qquad g = (g',\ g'+1\ \ldots\ M) \qquad \text{(II-14)}$$

for $N+1 \leq g' \leq M$.

Thus a particle in group g' may transfer into any group $g \geq g'$* for which the transfer probability is not zero. Such a transition from a neutron group, $1 \leq g' \leq N$, to a gamma-ray group $N+1 \leq g \leq M$ marks the end of a neutron history and the beginning of a gamma-ray history.

Importance sampling is then applied to the secondary gamma-ray production when the problem is performed in this manner by altering the p.d.f. for the selection of outgoing groups such that more important groups are selected more often. Assuming that a reasonable importance function $I_g(\bar{r})$ is known that measures the importance of group g relative to all other groups, the selection of the outgoing group g_o is made according to the altered set of group-to-group transfer probabilities defined by

$$\frac{P^{g\leftarrow g'}(\bar{r}) \times I_g(\bar{r})}{\sum_{g=g'}^{M} P^{g\leftarrow g'}(\bar{r}) \times I_g(\bar{r})}, \qquad g = (g',g'+1,\ldots M), \qquad \text{(II-15)}$$

*Group numbers usually increase with decreasing energy; however, $g \geq g'$ does not imply that the transfer must be from a higher energy to a lower energy since some gamma-ray energy groups may be higher in energy than the neutron energy group from which the particle transfers.

and the particle is given the weight $W_{g_o}(\bar{r})$ where

$$W_{g_o}(\bar{r}) = W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r}) + \Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \times \frac{\sum_{g=g'}^{M} P^{g\leftarrow g'}(\bar{r}) \times I_g(\bar{r})}{I_{g_o}(\bar{r})} \qquad \text{(II-16)}$$

for $1 \leq g' \leq N$,

$$W_{g_o}(\bar{r}) = W_{g'}(r) \times \frac{\Sigma_{s_\gamma}^{g'}(\bar{r})}{\Sigma_{t_\gamma}^{g'}(\bar{r})} \times \frac{\sum_{g=g'}^{M} P^{g\leftarrow g'}(\bar{r}) \times I_g(\bar{r})}{I_{g_o}(\bar{r})} \qquad \text{for } N+1 \leq g' \leq M \ . \qquad \text{(II-17)}$$

When the coupled problem is handled in this manner, at each collision the outgoing particle is given the statistical weight of the incoming particle times the appropriate nonabsorption weight adjustment as well as the weight adjustment due to energy biasing.

Method II: Combined Problem as a Dual Particle Problem with Altered Gamma Ray Generation Probabilities

A more conventional Monte Carlo method of solving the combined problem is to treat the neutron and secondary gamma rays separately in the random walk. In this case when a gamma ray is produced the neutron history is not necessarily terminated. For example, this would be true in analog Monte Carlo for a neutron inelastic scattering or biased Monte Carlo for nonabsorption weighting of the neutron. Thus when a secondary gamma ray is generated, its source position, group, and weight must be stored in a gamma-ray source bank or on a source tape for future processing and the neutron history is continued. The probability for secondary gamma-ray production by a neutron in group g' is given by the previously

defined cross-section ratio $\Sigma_{c_n}^{g'}(\bar{r})/\Sigma_{t_n}^{g'}(\bar{r})$ excluding the multiplicity factor. At every neutron collision a secondary gamma ray is either produced or not according to this gamma-ray generation probability. The gamma ray is given the precollision statistical weight of the neutron if it is produced and an energy group is selected from the normalized p.d.f. which is the set of discrete neutron group-to-gamma-ray group transfer probabilities given by

$$\frac{\int \Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')\,d\bar{\Omega}}{\Sigma_{c_n}^{g'}(\bar{r})}\ , \quad (g = N+1, N+2, \ldots M) \quad . \tag{II-18}$$

Importance sampling may be applied to secondary gamma-ray production when the coupled problem is run in this manner by altering the natural gamma-ray production probability based on an importance function $I_g(\bar{r})$.

Initially an outgoing gamma-ray group g is selected from the p.d.f. given above at every neutron collision in group g'. Then a new gamma-ray generation probability is formed from $I_g(\bar{r})$ which relates the importance of a gamma ray in group g which has weight

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \tag{II-19}$$

to the importance of a neutron in group g' which has weight

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \quad . \tag{II-20}$$

where $W_{g'}(\bar{r})$ is the weight of the incoming neutron. This new function $H_{g,g'}(\bar{r})$ is given by

$$H_{g,g'}(\bar{r}) = \frac{I_g(\bar{r}) \times \Sigma_{c_n}^{g'}(\bar{r})}{I_g(\bar{r}) \times \Sigma_{c_n}^{g'}(\bar{r}) + I_{g'}(\bar{r}) \times \Sigma_{s_n}^{g'}(\bar{r})} \quad . \tag{II-21}$$

At every neutron collision in group g' a gamma ray is either produced in energy group g or is not produced according to the new generation probability $H_{g,g'}(\bar{r})$.

If a gamma ray is produced, its statistical weight is given by

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})/\Sigma_{t_n}^{g'}(\bar{r})}{H_{g,g'}(\bar{r})} \quad . \tag{II-22}$$

With this procedure, the average weight leaving a neutron collision is given by the weight of the incoming neutron times the probability of the neutron not being absorbed plus the weight of the outgoing gamma ray times the probability it is produced or

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} + W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})/\Sigma_{t_n}^{g'}(\bar{r})}{H_{g,g'}(\bar{r})} \times H_{g,g'}(\bar{r}) \tag{II-23}$$

$$= W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} + W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \quad .$$

which is equal to the average weight leaving a neutron collision in the analog case.

Method III: Combined Problem as a Dual Particle Problem with Russian Roulette and Splitting

Yet another method of applying importance sampling to the production of secondary gamma rays is by the use of Russian roulette and splitting to decrease or increase respectively the number of samples in any region of phase space. These techniques may be considered as a form of survival biasing by which unimportant gamma rays are terminated with some probability or an important gamma ray is multiplied to give several semi-independent gamma rays. This method requires that initially a gamma ray be produced at every neutron collision in group g' by requiring the gamma-ray weight $W_g(\bar{r})$ to be given by

$$W_g(\bar{r}) = W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \qquad \text{(II-24)}$$

where $W_{g'}(r)$ is the weight of the incoming neutron and the multiplicity of gamma rays included in the gamma-ray generation probability accounts for more than one gamma ray being produced in the collision process. The outgoing gamma-ray group g is then selected from the set of discrete neutron group to gamma-ray group transfer probabilities given in Equation (II-18).

Russian roulette and splitting are now applied to this gamma ray to produce gamma rays of the desired weight standard $V_g(\bar{r})$. That is, if the gamma-ray weight, $W_g(\bar{r})$, is less than $V_g(\bar{r})$, then Russian roulette is applied such that this gamma-ray history is continued with probability

$$\frac{W_g(\bar{r})}{V_g(\bar{r})} \tag{II-25}$$

or terminated with probability

$$1 - \frac{W_g(\bar{r})}{V_g(\bar{r})} \quad . \tag{II-26}$$

However, if the gamma-ray weight is greater than $V_g(\bar{r})$, then splitting is applied such that there are G (integer) gamma rays generated where

$$G = \text{whole part of } \frac{W_g(\bar{r})}{V_g(\bar{r})} \tag{II-27}$$

and Russian roulette is played with the remaining weight

$$W_g(\bar{r}) - G \times V_g(\bar{r}) \quad . \tag{II-28}$$

All of the gamma rays so produced receive the weight standard $V_g(\bar{r})$ to account for this biased sampling.

In order to show that such a procedure is valid, it is necessary to consider the average weight leaving a neutron collision in each of the above cases. First consider Russian roulette where the average weight leaving a collision is the sum of the neutron weight and gamma-ray weight multiplied by these respective production probabilities

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}(\bar{r})} + V_g(\bar{r}) \times \frac{W_g(\bar{r})}{V_g(\bar{r})} \tag{II-29}$$

$$= W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}(\bar{r})} + W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{c_t}^{g'}(\bar{r})} \quad .$$

This is the average value of the weight leaving a neutron collision in the analog case.

Now consider the combination of splitting and Russian roulette where the average weight leaving a neutron collision is the sum of the neutron weight, the weight of the gamma rays generated by splitting and the weight of the gamma ray generated by Russian roulette times their respective production probabilities:

$$W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} + G \times V_g(\bar{r}) + V_g(\bar{r}) \times \frac{W_g(\bar{r}) - G \times V_g(\bar{r})}{V_g(\bar{r})} \tag{II-30}$$

$$= W_{g'}(\bar{r}) \times \frac{\Sigma_{s_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} + W_{g'}(\bar{r}) \times \frac{\Sigma_{c_n}^{g'}(\bar{r})}{\Sigma_{t_n}^{g'}(\bar{r})} \quad .$$

Again the average weight leaving a collision is as in the analog case.

In order for this method of importance sampling to be effective, the weight standards must be so chosen that important gamma rays are produced and unimportant gamma rays are killed. It is obvious that these weight standards must be related to the importance function I(P). This relationship can be obtained by consideration of a special case in which the relationship between the particle weight and the adjoint function is known, namely at the source. In terms of the adjoint matrix J(P), λ is given by[6]

$$\lambda = \int S^T(P)\ J(P)dP \tag{II-31}$$

where $S^T(P)$ is the transpose of S(P). Assuming the source to be defined

as isotropic in group g_o and located at space point r_o,

$$\lambda = S_{g_o}(\bar{r}_o) \times J_{g_o}(\bar{r}_o) \quad . \tag{II-32}$$

The initial weight of a particle $W_{g_o}(\bar{r}_o)$ can be equated to the source and the importance function $I_{g_o}(\bar{r}_o)$ with the adjoint function with the result

$$W_{g_o}(\bar{r}) = \frac{\lambda}{I_{g_o}(r_o)} \quad . \tag{II-33}$$

Thus the particle weight is given by the reciprocal of the importance function times the effect of interest. This relationship holds at any point in phase space for an optimum method of importance sampling using density biasing.[5] This method makes use of the exact adjoint solution J(P) to modify the source S(P) and the transition kernel K(P←P') and can be combined with "last event" estimation to yield answers completely free of statistical fluctuations,[7] i.e., all histories give the exact same estimate of the effect of interest. One of the results of this optimum method of biasing is that at any point in phase space the weight of the particles times the corresponding adjoint flux is equal to the effect of interest. This implies then that optimum weight standards for secondary gamma rays are to be calculated according to

$$V_g(\bar{r}) = \frac{\lambda}{J_g(\bar{r})} \tag{II-34}$$

where approximate values of λ and $J_g(\bar{r})$ can be obtained from an adjoint solution to a simplified version of the problem under investigation. (It is obvious if the exact adjoint solution were known λ could be obtained directly from equation II-31.)

Source Angle Biasing of Secondary Gamma Rays

The methods of biasing secondary gamma rays in energy and space which have been developed in the previous section were based on the importance function $I_g(\bar{r})$. The extension of these methods to include source angular biasing of the secondary gamma rays requires only that an importance function $I_g(\bar{r},\bar{\Omega})$ be available which is the angular importance of a gamma ray in energy group g and at space point $\bar{r}$. The normalized p.d.f. for the selection of an outgoing direction $\bar{\Omega}$ of a secondary gamma ray in group g produced by a neutron collision in group g' is given by

$$\frac{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r})} \quad . \tag{II-35}$$

In order to bias the selection of the outgoing gamma-ray direction, selection is made from the altered p.d.f. given by

$$\frac{\dfrac{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r})} \times I_g(\bar{r},\bar{\Omega})}{\displaystyle\int \frac{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r})} \times I_g(\bar{r},\bar{\Omega})\,d\bar{\Omega}} \quad . \tag{II-36}$$

For a gamma ray of weight $W_g(\bar{r})$ the weight adjustment is given by

$$W_g(\bar{r}) \times \frac{\displaystyle\int \frac{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}'')}{\Sigma_{c_n}^{g\leftarrow g'}(\bar{r})} \times I_g(\bar{r},\bar{\Omega})\,d\bar{\Omega}}{I_g(r,\bar{\Omega}_o)} \tag{II-37}$$

where $\overline{\Omega}_o$ is the outgoing direction selected. To select from this altered distribution $\Sigma_{c_n}^{g\leftarrow g'}(\overline{r},\overline{\Omega}\leftarrow\overline{\Omega}'')$ and $I_g(\overline{r},\overline{\Omega})$ must be in terms of the same coordinate system. However, the angular distribution of $\Sigma_{c_n}^{g\leftarrow g'}(\overline{r},\overline{\Omega}\leftarrow\overline{\Omega}'')$ is specified relative to the incoming neutron direction $\overline{\Omega}''$ and is assumed to be azimuthally symmetric about this direction whereas $I_g(\overline{r},\overline{\Omega})$ would usually be given in terms of the laboratory coordinate system. This complication is avoided if the source angular distribution of secondary gamma rays is assumed to be isotropic. Then the natural angular distribution is symmetric about all directions and the normalized p.d.f.

$$\frac{\Sigma_{c_n}^{g\leftarrow g'}(\overline{r},\overline{\Omega}\leftarrow\overline{\Omega}'')}{\Sigma_{c_n}^{g\leftarrow g'}(\overline{r})} = \frac{1}{4\pi} \quad . \tag{II-38}$$

The altered p.d.f becomes

$$\frac{I_g(\overline{r},\overline{\Omega})}{\int I_g(\overline{r},\overline{\Omega})\,d\overline{\Omega}} \tag{II-39}$$

and the weight adjustment is given by

$$W_g(\overline{r}) \quad \times \quad \frac{\frac{1}{4\pi}\int I_g(\overline{r},\overline{\Omega})\,d\overline{\Omega}}{I_g(r,\Omega_o)} \quad . \tag{II-40}$$

CHAPTER III

PRESENTATION AND DISCUSSION OF RESULTS

The three methods of secondary gamma-ray importance sampling described in Chapter II were studied using a modified version of the Monte Carlo code MORSE.[1] These modifications allowed for the various biasing techniques of the secondary gamma-ray generation to be incorporated into the random walk subroutines of the code as well as for secondary gamma-ray source angle biasing.

The problem considered was the determination of the tissue dose due to gamma rays at the outside surface of a 200-cm-thick concrete slab shield. Two source conditions were considered: (1) a 14-MeV neutron beam source and (2) an isotropic ^{235}U fission source. MORSE calculations were performed for these source conditions employing each of the three secondary gamma-ray production biasing techniques to be evaluated. Calculations using the method* of biasing the secondary gamma-ray production employed by the standard MORSE code were also performed for the 14-MeV and fission source cases to be used as a basis for evaluating the other three methods. In the standard method the gamma-ray generation probabilities as a function of position and energy groups were simply estimated based on what regions and energy groups were thought to be important. The problem was then treated as in Method II using these estimated values as the gamma-ray generation probabilities. It is this procedure of having to estimate the biasing parameters that the new methods

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*Hereafter this method will be referred to as the "standard method."

developed here will eliminate as well as to provide secondary gamma-ray biasing techniques which make use of a detailed importance function.

As a further check on the validity of these new biasing techniques, the results of all the calculations were compared with those obtained with the discrete ordinates code ANISN.[2]

Calculation Details

All of the MORSE calculations included not only the biasing particular to one of the gamma-ray generation techniques but also secondary gamma-ray source angle biasing, neutron and gamma-ray path length stretching, neutron and gamma-ray nonabsorption weighting and neutron and gamma-ray Russian roulette.

The biasing parameters for path length stretching were obtained from the code BIASPREP.[8] Additional subroutines were added to this code to provide the biasing parameters averaged over spatial regions for importance sampling the secondary gamma-ray generation as well as for secondary gamma-ray source angle biasing. This included region averaged values of the importance function $I_g(\bar{r})$ to be used with biasing Methods I and II, region averaged weight standards $V_g(\bar{r})$ to be used with Method III, and region averaged values of the importance function $I_g(\bar{r},\bar{\Omega})$ to be used for the source angle biasing. In all of the MORSE calculations these parameters were obtained for five equal spatial regions (40-cm-thick) extending across the concrete slab.

The basic function of the BIASPREP code is to prepare these biasing parameters for input into the MORSE code using a precalculated importance function. The importance function used in the present work was the

coupled adjoint flux solution to the concrete shield problem obtained from the discrete ordinates code ANISN. Since the effect of interest was the gamma-ray dose at the outside surface of the shield, the source for the ANISN adjoint problem was specified as isotropic at this outside surface and with a magnitude equal to the gamma-ray fluence-to-dose factors (Table III-1). As the ANISN adjoint calculation was a coupled problem, the adjoint flux solution was obtained for both neutrons and gamma-ray groups.

One-dimensional slab geometry was used to represent the 200-cm-thick concrete shield in both the MORSE and ANISN calculations. The spatial mesh in the ANISN calculations consisted of 100 intervals 2-cm wide. The gamma-ray tissue dose was calculated at each of these mesh intervals for both the forward and adjoint ANISN calculations. An S_{16} angular quadrature was used for all discrete ordinates calculations.

In the MORSE calculation, boundary crossing estimators[9] were used to calculate the gamma-ray dose at 40, 80, 120, and 160 cm from the source. The dose at the outside surface of the shield (200 cm) was calculated using next-event estimation.[9]

Cross-Section Preparation

Both the Monte Carlo and the discrete ordinates calculations used an identical set of coupled multigroup cross sections which employ 22 neutron groups and 18 gamma-ray groups. The energy group limits defining these 40 groups are given in Table III-1 along with the corresponding group-averaged fluence-to-dose response functions used to calculate the tissue dose.

TABLE III-1

Energy Group Structure for Coupled Multigroup Cross Sections
40 Groups

Group Number	Upper Energy (eV)	Tissue Dose Response Function[10] (rads/particle/cm^2)
Neutron Groups		
1	1.50(+7)[a]	5.46(-9)
2	1.22(+7)	5.13(-9)
3	1.00(+7)	4.84(-9)
4	8.19(+6)	4.61(-9)
5	6.36(+6)	4.44(-9)
6	4.97(+6)	4.13(-9)
7	4.07(+6)	4.01(-9)
8	3.01(+6)	3.39(-9)
9	2.46(+6)	3.15(-9)
10	2.35(+6)	3.09(-9)
11	1.83(+6)	2.64(-9)
12	1.11(+6)	1.97(-9)
13	5.50(+5)	1.12(-9)
14	1.10(+5)	2.29(-10)
15	3.35(+3)	0.0
16	5.83(+2)	0.0
17	1.01(+2)	0.0
18	2.90(+1)	0.0
19	1.06(+1)	0.0
20	3.05	0.0
21	1.12	0.0
22	4.14(-1)[b]	0.0
Gamma-Ray Groups		
23	1.00(+7)	2.49(-9)
24	8.00(+6)	2.02(-9)
25	6.50(+6)	1.71(-9)
26	5.00(+6)	1.44(-9)
27	4.00(+6)	1.20(-9)
28	3.00(+6)	1.01(-9)
29	2.50(+6)	8.70(-10)
30	2.00(+6)	7.48(-10)
31	1.66(+6)	6.48(-10)
32	1.33(+6)	5.34(-10)
33	1.00(+6)	4.30(-10)
34	8.00(+5)	3.48(-10)
35	6.00(+5)	2.56(-10)
36	4.00(+5)	1.79(-10)
37	3.00(+5)	1.24(-10)
38	2.00(+5)	6.86(-11)
39	1.00(+5)	3.64(-11)
40	5.00(+4)	8.55(-11)
	2.00(+4)[c]	

[a]Read as 1.50×10^7.
[b]Thermal neutron group.
[c]Lower limit of gamma-ray group 40.

The form of these cross sections is basically a set of four 40 by 40 group-to-group transfer matrices denoted P_0, P_1, P_2, and P_3. This set of four matrices (referred to as a P_3 cross-section set) is a result of approximating the angular dependence of the neutron elastic scattering cross section and the gamma-ray Compton scattering cross section for a given group-to-group transfer with third-order Legendre polynomial expansions. Neutron-to-neutron energy group transfers as a result of neutron reactions other than elastic and gamma-ray-to-gamma-ray energy group transfers as a result of gamma-ray reactions other than Compton scattering appear as part of the transfer cross sections only in the P_0 matrix since such reactions were assumed to take place isotropically in the laboratory coordinate system. This is also true for neutron group to gamma-ray group energy transfers since the secondary gamma rays were also assumed to be emitted isotropically in the laboratory coordinate system.

These multigroup transfer cross-section matrices were formed from point cross-section data for each of the eleven elements of the concrete composition given in Table III-2. Initially, 104 group P_3 neutron cross-section sets were generated for each element with the cross-section code SUPERTOG[11] using a 1/E flux weighting. Similarly, 18 group, P_3, gamma-ray cross-section sets were generated with the cross-section code MUG[12] using a constant or flat weighting.

The P_3 neutron cross-section sets were further reduced to 22 neutron groups by weighting with the flux obtained from a 104-group ANISN calculation for a fission source in an infinite medium of concrete.

Table III-2

Concrete Composition[a]

Element	Density[b] (atoms/b-cm)	Source of Cross-Section Data
H	8.9326(-3)[c]	Ref. 14
O	4.0015(-2)	Ref. 14
Na	1.0725(-3)	Ref. 14
Mg	2.1055(-3)	Ref. 14
Al	3.0557(-3)	Ref. 14
Si	1.0591(-2)	Ref. 15
K	2.3103(-4)	Ref. 16
Ca	4.4345(-3)	Ref. 16
Ti	1.3835(-4)	Ref. 14
Mn	3.2870(-5)	Ref. 14
Fe	1.9204(-3)	Ref. 14

[a]Type O-HW1 ordinary concrete excluding P and S (see ref. 13).

[b]Density of composition = 2.328 grams/cm^3.

[c]Read as 8.9326×10^{-3}.

Secondary gamma-ray production cross sections were prepared as group-to-group transfers from the 22 neutron groups to the 18 gamma-ray groups by the cross-section code POPOP4.[17] These secondary gamma-ray production cross sections along with the P_3 neutron cross-section sets and the P_3 gamma-ray cross-section set were then input to the COUPLING[18] code to produce a coupled, P_3, cross-section set for each of the eleven elements.

These coupled sets were then converted from microscopic to macroscopic cross sections with the code JRMACRO[19] by weighting each element by its atom density in concrete (Table III-1) to give the coupled P_3 concrete cross-section set used in the MORSE and ANISN calculations.

Calculation Results

The results of the MORSE Monte Carlo calculations are compared with the ANISN discrete ordinates calculation in Figures III-1 through III-8. Figure III-1 through Figure III-4 show the gamma-ray dose as a function of distance into the concrete slab for each of the three secondary gamma-ray generation importance sampling methods and the standard method for the 14-MeV source case, while Figures III-5 through III-8 show the same results for the fission source case. (The fraction of source particles in the neutron groups for the ^{235}U fission source is given in Table III-3.)

In general, all of the Monte Carlo results agreed well with the ANISN results. However, in each of the calculations the ANISN results fell outside the statistics of the MORSE results for at least one of

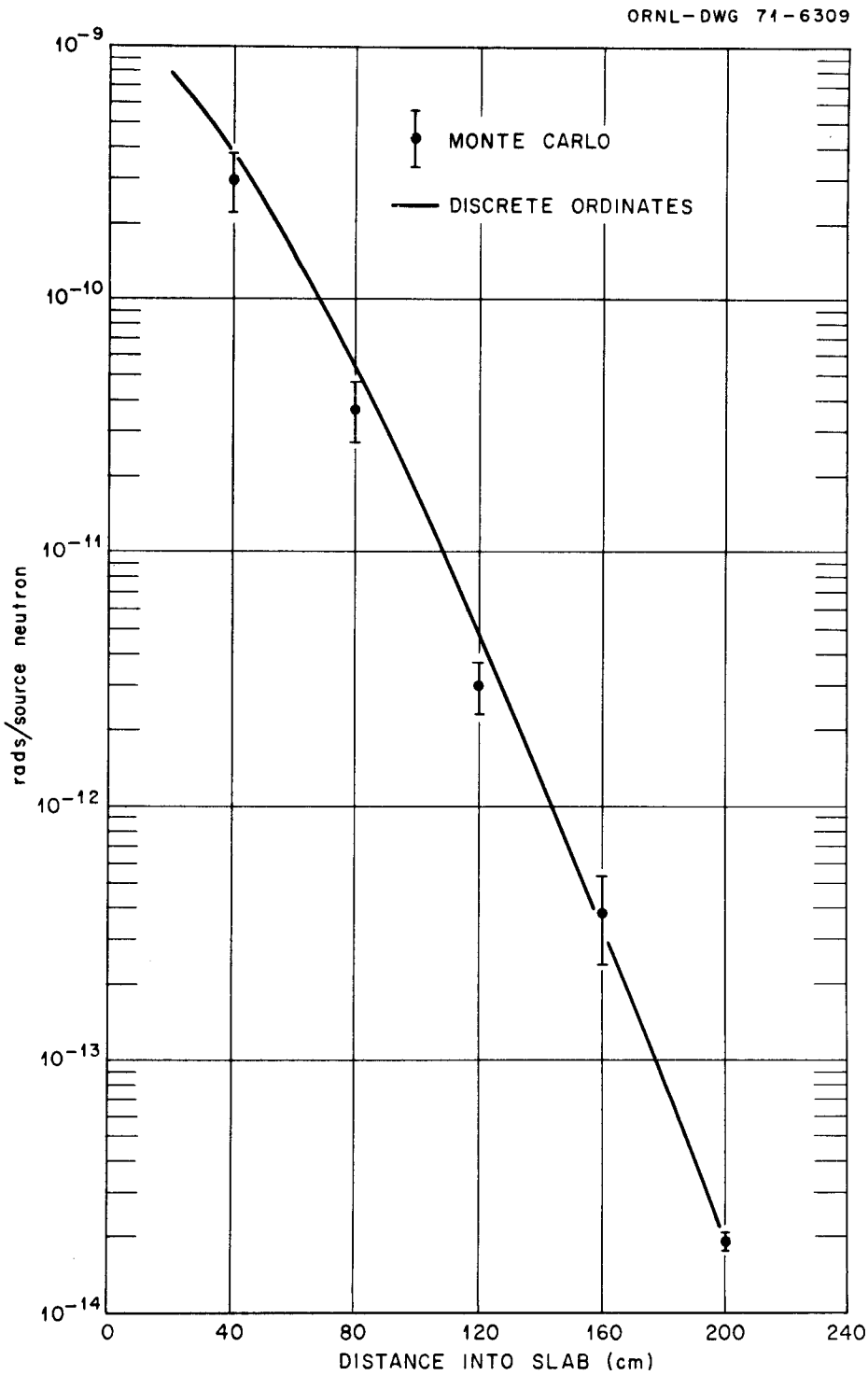

Fig. III-1. Gamma-Ray Tissue Dose vs Distance into Slab for 14-MeV Source (Importance Sampling Method I).

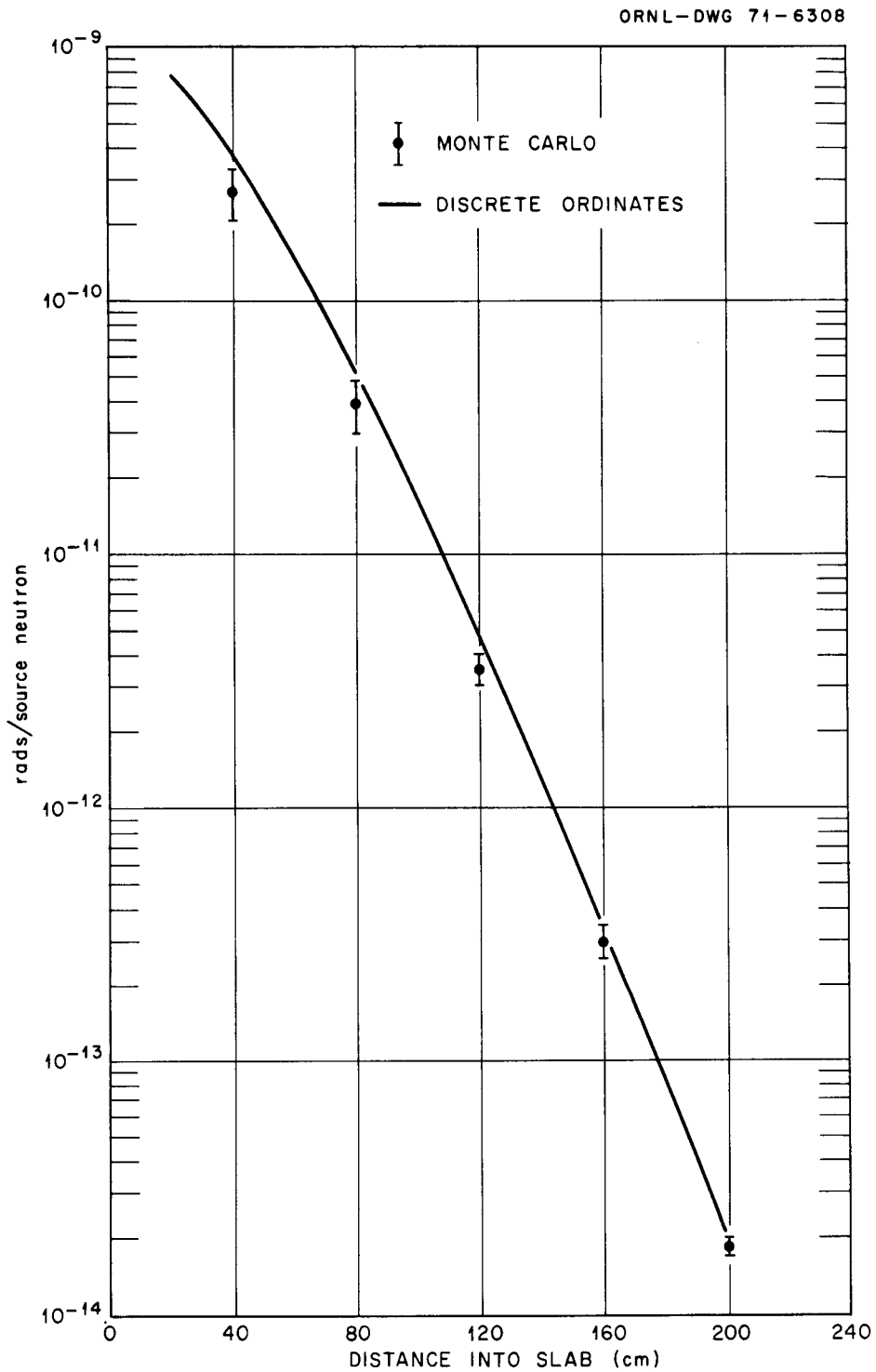

Fig. III-2. Gamma-Ray Tissue Dose vs Distance into Slab for 14-MeV Source (Importance Sampling Method II).

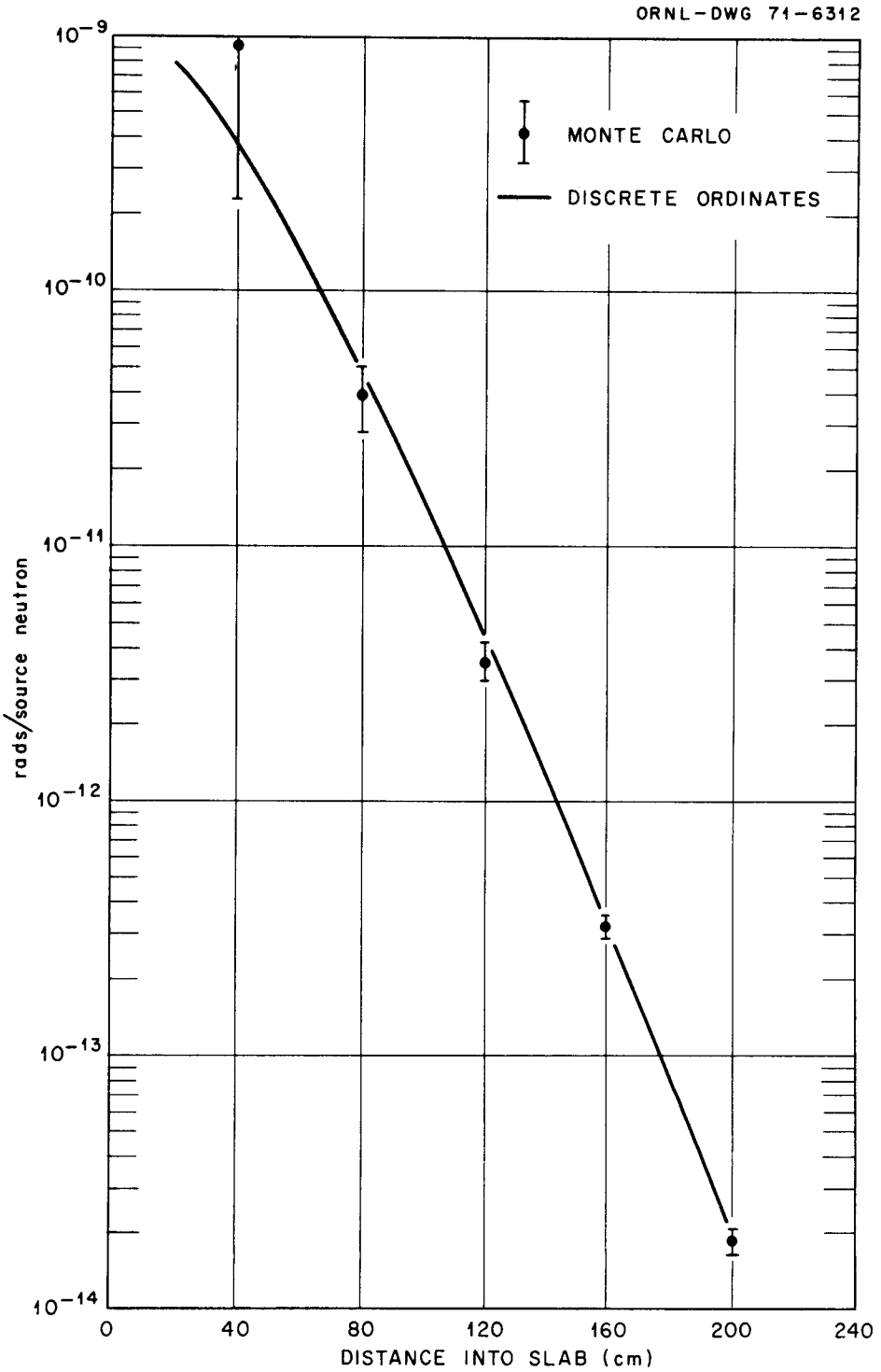

Fig. III-3. Gamma-Ray Tissue Dose vs Distance into Slab for 14-MeV Source (Importance Sampling Method III).

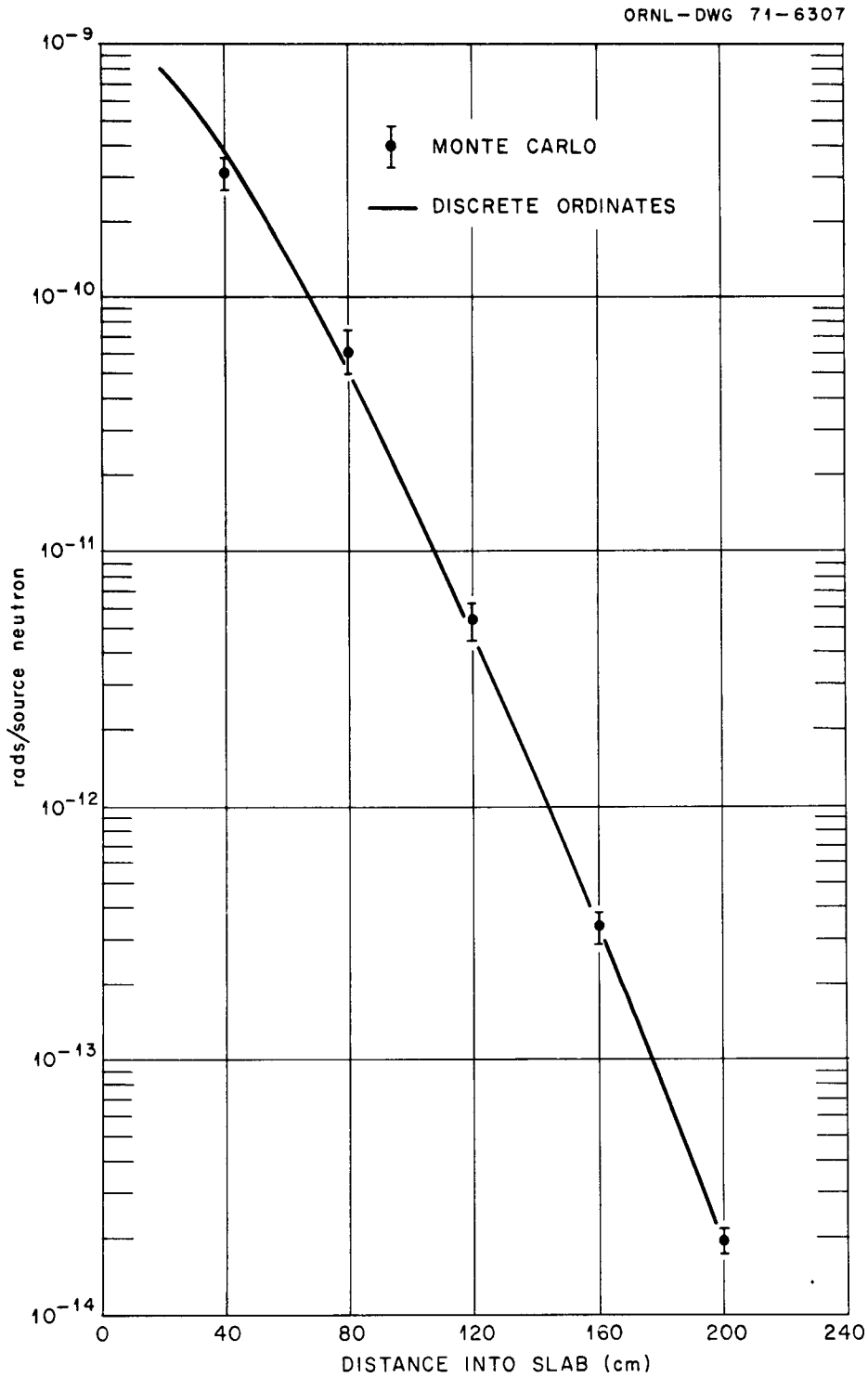

Fig. III-4. Gamma-Ray Tissue Dose vs Distance into Slab for 14-MeV Source (Standard Method).

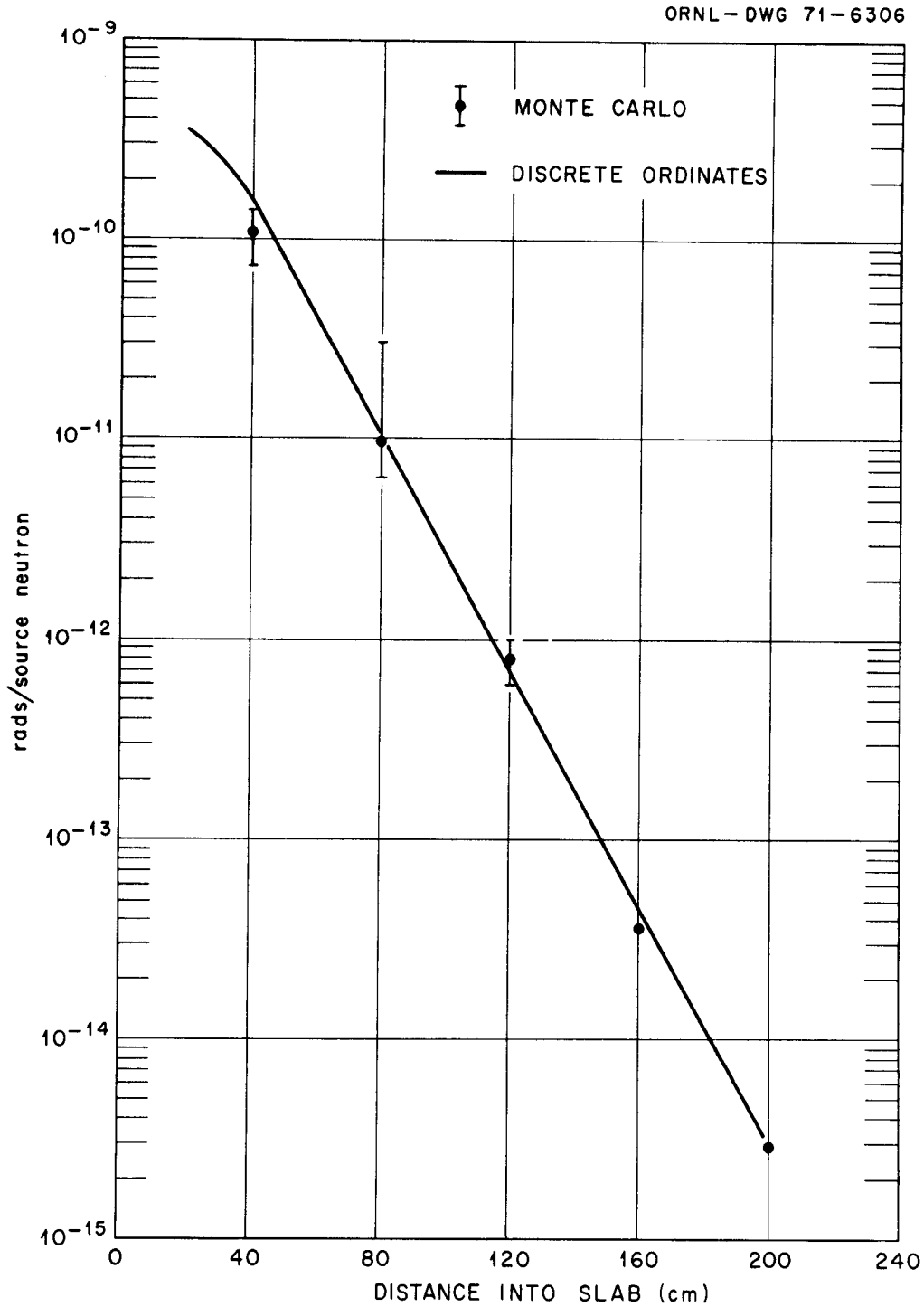

Fig. III-5. Gamma-Ray Tissue Dose vs Distance into Slab for Fission Source (Importance Sampling Method I).

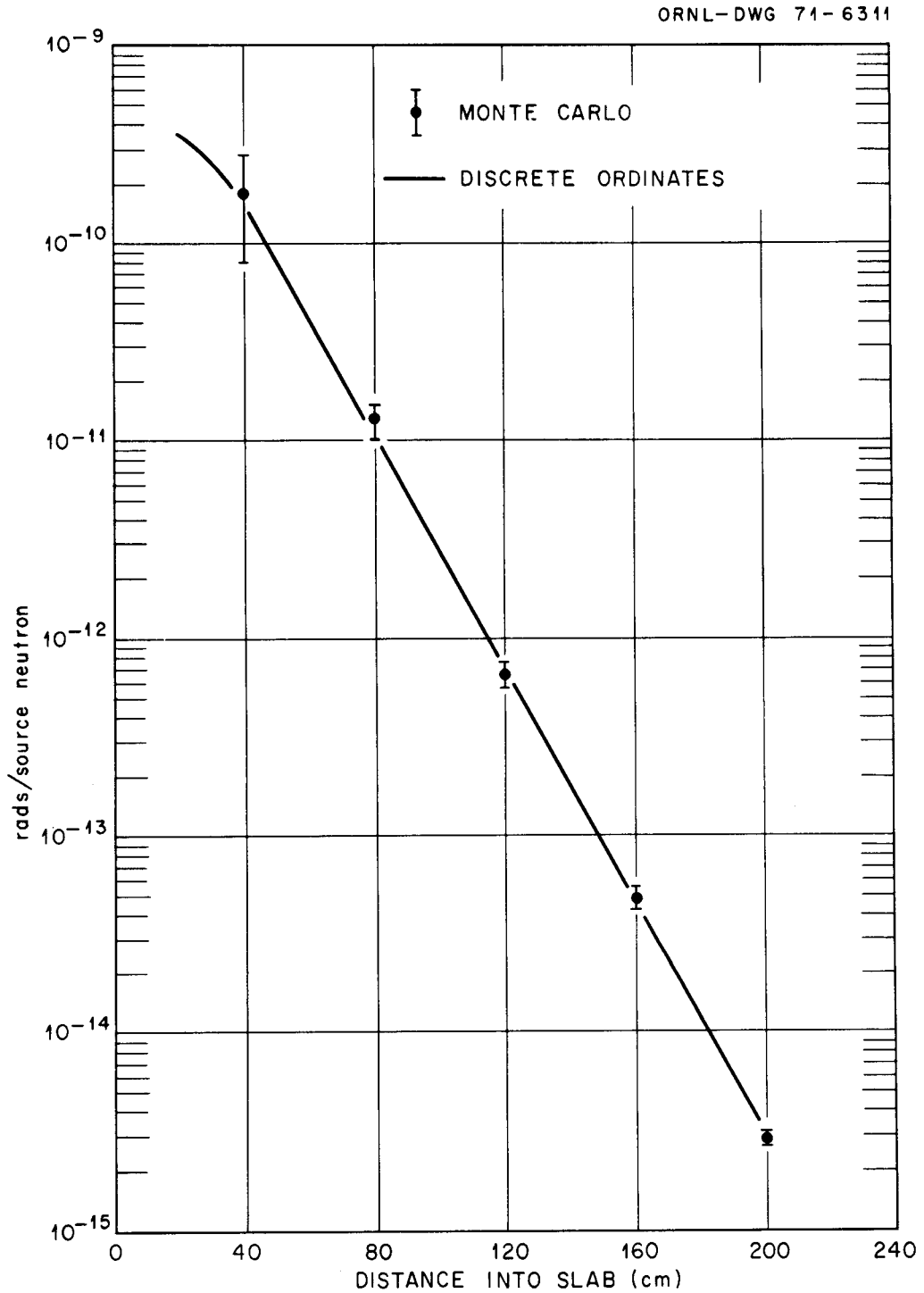

Fig. III-6. Gamma-Ray Tissue Dose vs Distance into Slab for Fission Source (Importance Sampling Method II).

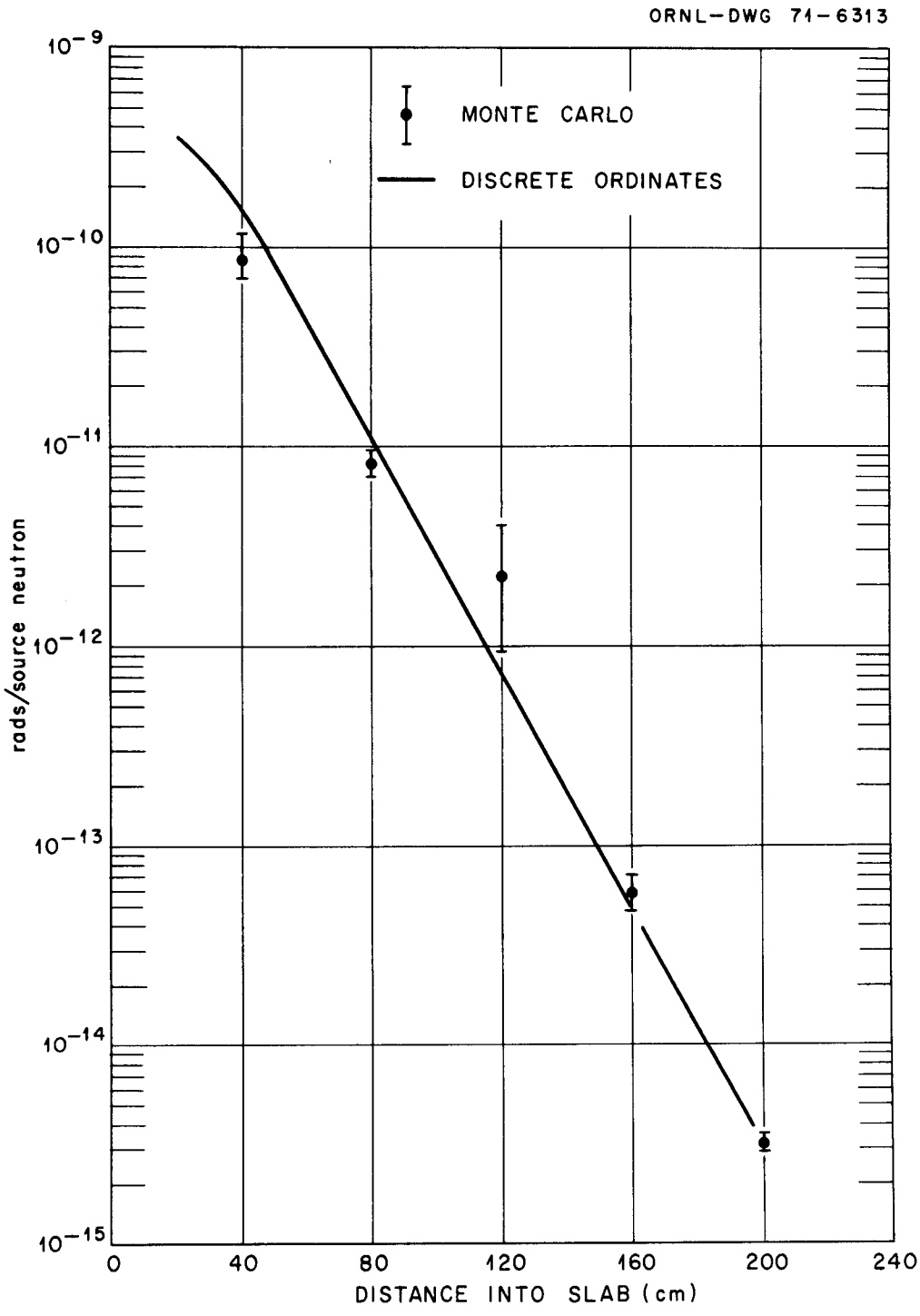

Fig. III-7. Gamma-Ray Tissue Dose vs Distance into Slab for Fission Source (Importance Sampling Method III).

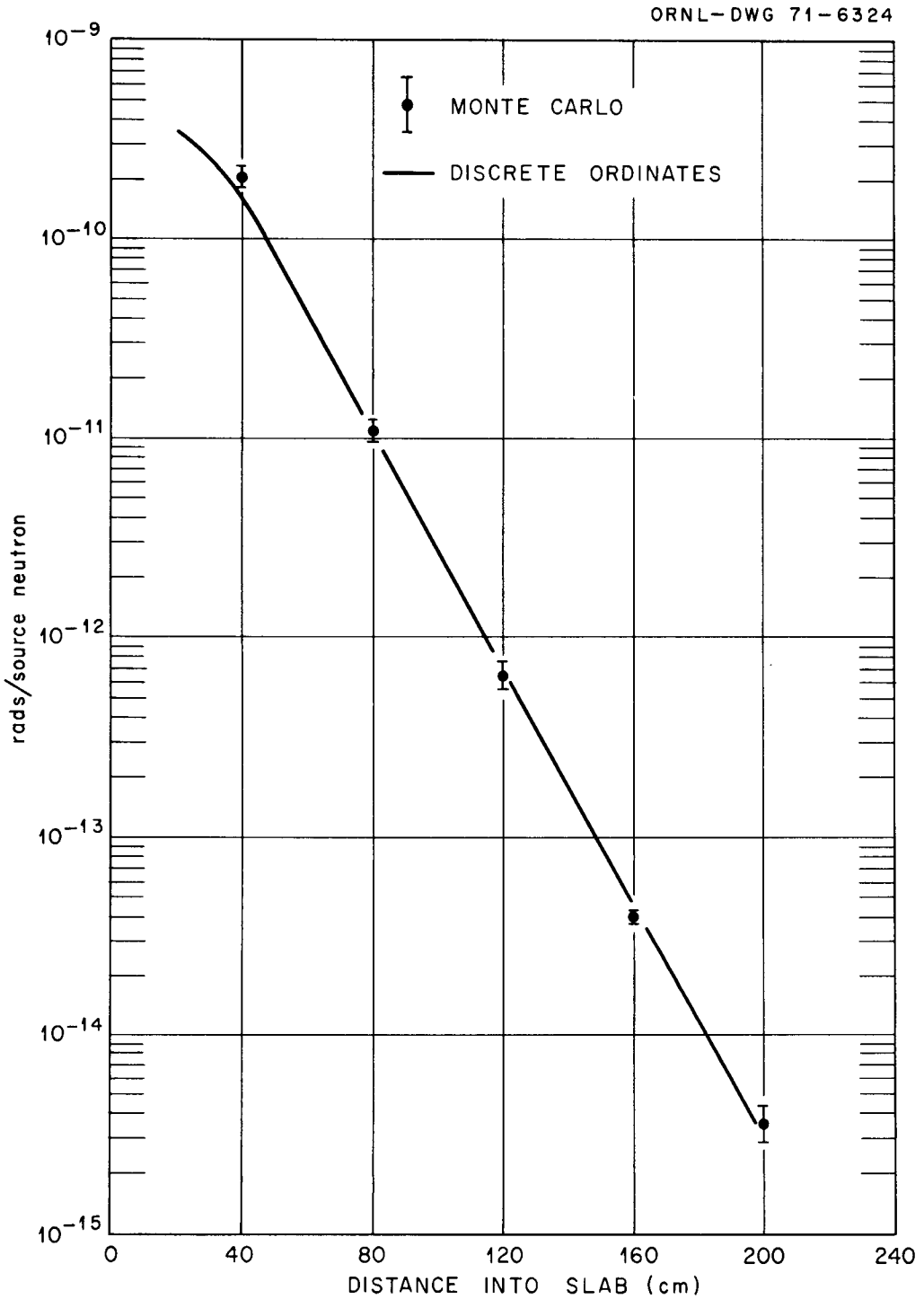

Fig. III-8. Gamma-Ray Tissue Dose vs Distance into Slab for Fission Source (Standard Method).

Table III-3

Energy Distributions for Fission Source

Energy (MeV)	Fraction of Particles in Group
12.2-15.0	1.568(-4)[a]
10.0-12.2	8.932(-4)
8.19-10.0	3.480(-3)
6.36-8.19	1.392(-2)
4.97-6.36	3.457(-2)
4.07-4.97	3.507(-2)
3.01-4.07	1.072(-1)
2.46-3.01	8.898(-2)
2.35-2.46	2.323(-2)
1.83-2.35	1.203(-1)
1.11-1.83	2.181(-1)
0.55-1.11	1.983(-1)
0.11-0.55	1.403(-1)
0.0335-0.110	1.550(-2)
5.83(-4)-3.35(-3)	0
1.01(-4)-5.83(-4)	0
2.90(-5)-1.01(-4)	0
<2.90(-5)	0

[a]Read as 1.568×10^{-4}.

the five detector points as can be observed by the error bars* on the Monte Carlo data points. It should be noted that the poorer statistics (larger error bars) were always associated with those detector points other than the last detector. This is a consequence of the biasing being designed to yield gamma-ray histories which contribute most heavily to the last detector and consequently the other detector regions are under-sampled. This general agreement with the ANISN results confirms the validity of these importance sampling procedures.

The comparison of the three methods of secondary gamma-ray importance sampling is given in Table III-4 in terms of the results obtained for the gamma-ray dose at the shield surface for the 14-MeV and fission sources.** For each calculation the estimated fractional standard deviation of the mean is given with a corresponding figure of merit. Following standard practice, the "figure of merit" is taken as the variance times the total computer computation time. This quantity is intended to express the relative value of the secondary gamma-ray importance sampling methods such that the smaller the figure of merit the better the method. For both the 14-MeV and fission source cases, Method I ranks as the best method followed by Method II, Method III, and the Standard Method in that order. The figure of merit indicates Method I to be a factor of 6.2 better than the Standard Method for the 14-MeV source case and a factor of 40.0 better for the fission source case. Method II is a factor of 2.2 better than the Standard Method for

*All error bars are one standard deviation. Data points with no error bars have a fractional standard deviation of less than 6%.

**ANISN results are also given in Table III-4.

Table III-4

Comparison of the Monte Carlo Results Obtained with the Various Secondary Gamma-Ray Importance Sampling Techniques for the Concrete Shield[a]

Importance Sampling Techniques	Number of Neutron Histories[b]	Number of Secondary Gamma Rays Generated	Gamma-Ray Tissue Dose at Shield Surface (rads/source neutron)	Fractional Standard Deviation of Mean	Figure[c] of Merit
			14-MeV Source		
Method I	8,000	5,864	1.92(-14)[d]	0.07	0.03
Method II	8,000	14,293	1.85(-14)	0.09	0.09
Method III	8,000	7,318	1.88(-14)	0.12	0.15
Standard	8,000	112,127	1.95(-14)	0.09	0.20
ANISN			1.94(-14)		
			Fission Source		
Method I	16,000	5,852	2.93(-15)	0.05	0.02
Method II	16,000	11,750	2.95(-15)	0.09	0.10
Method III	16,000	14,649	3.20(-15)	0.10	0.13
Standard	16,000	101,311	3.64(-15)	0.20	0.84
ANISN			3.20(-15)		

[a] ANISN results are also included in the comparison.

[b] These neutron histories were divided into 40 equal batches for each calculation.

[c] Figure of Merit = (variance) × (IBM 360/91 computer time in minutes).

[d] Read as: 1.92×10^{-14}.

the 14-MeV source case and a factor of 8.5 better for the fission source case. Finally Method III is a factor of 1.3 better than the Standard Method in the 14-MeV source case and a factor of 6.6 better in the fission source case.

It should be noted that the figure of merit does not take into account the deviation of the Monte Carlo results from those obtained with ANISN which are taken to be the true answer in this one-dimensional problem. However, the results for the gamma-ray dose calculations at the shield surface (last detector) for each of the MORSE calculations compared, within statistics, with the ANISN result except in the fission source case using importance sampling Method I. In this case the MORSE result is 9% lower than the ANISN result but with a fractional standard deviation of only 5%.

Spatial Distribution of Secondary Gamma-Ray Generations

Figures III-9, III-10, and III-11 show the spatial distribution of these secondary gamma-ray generations throughout the concrete slab using importance sampling Methods I, II, and III respectively for the 14-MeV source case. Each point on the graph represents the location of a secondary gamma-ray generation in the concrete. The 14-MeV neutron source is located at the origin (0,0) of the graphs. The total number of secondary gamma rays generated in each of the calculations is listed in Table III-4.

The spatial distribution of the gamma-ray generations is very similar for Methods I and II, although less than half as many gamma rays were generated in Method I as compared to Method II for the same

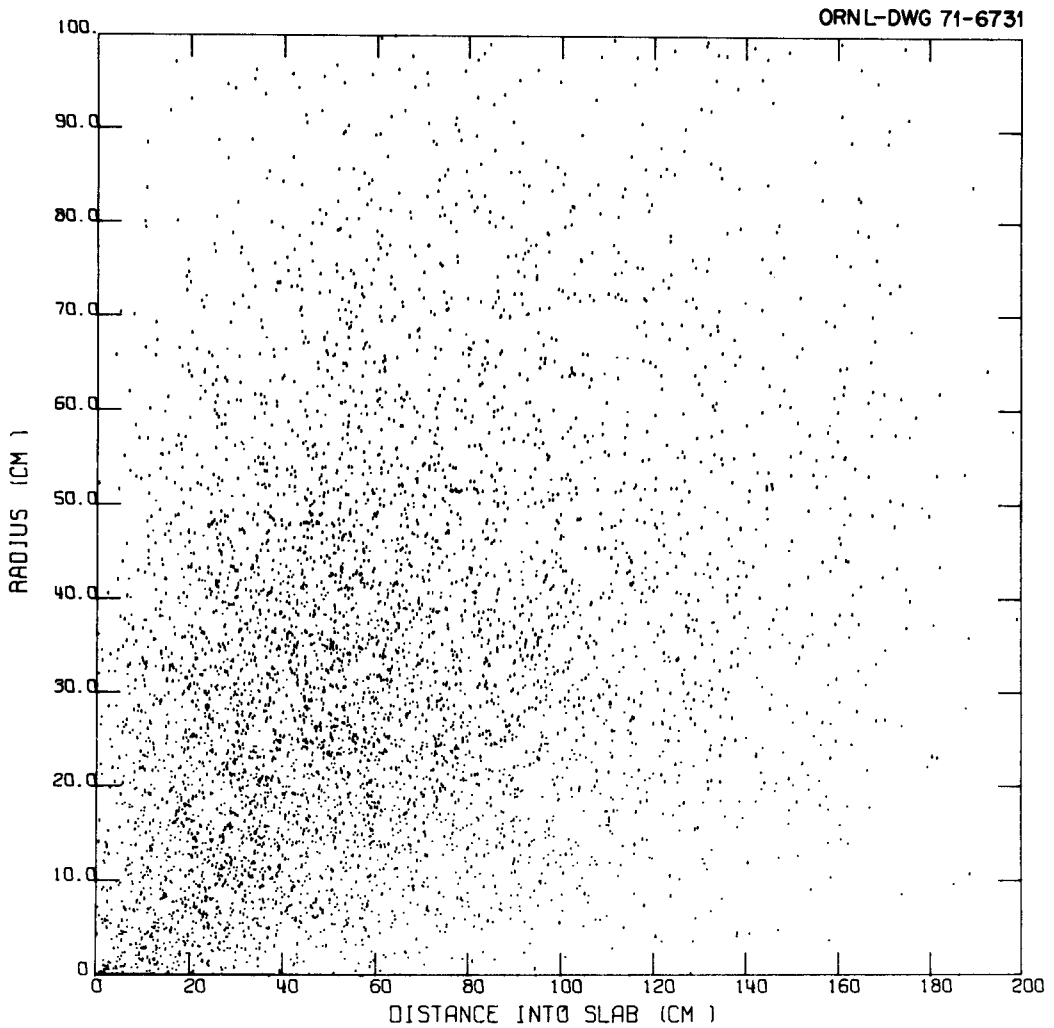

Fig. III-9. Distribution of Secondary Gamma-Ray Generations in Slab for 14-MeV Source Located at Origin (Importance Sampling Method I).

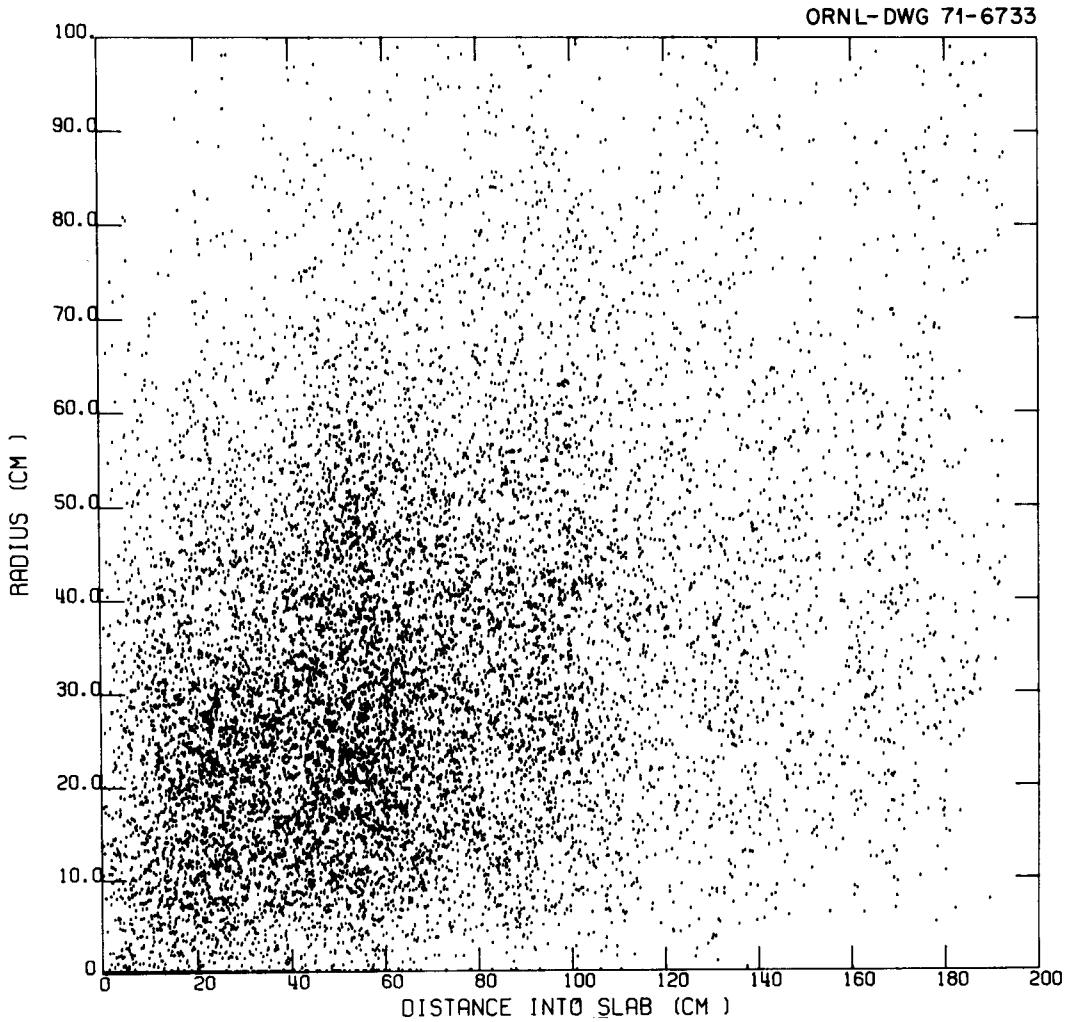

Fig. III-10. Distribution of Secondary Gamma-Ray Generations in Slab for 14-MeV Source Located at Origin (Importance Sampling Method II).

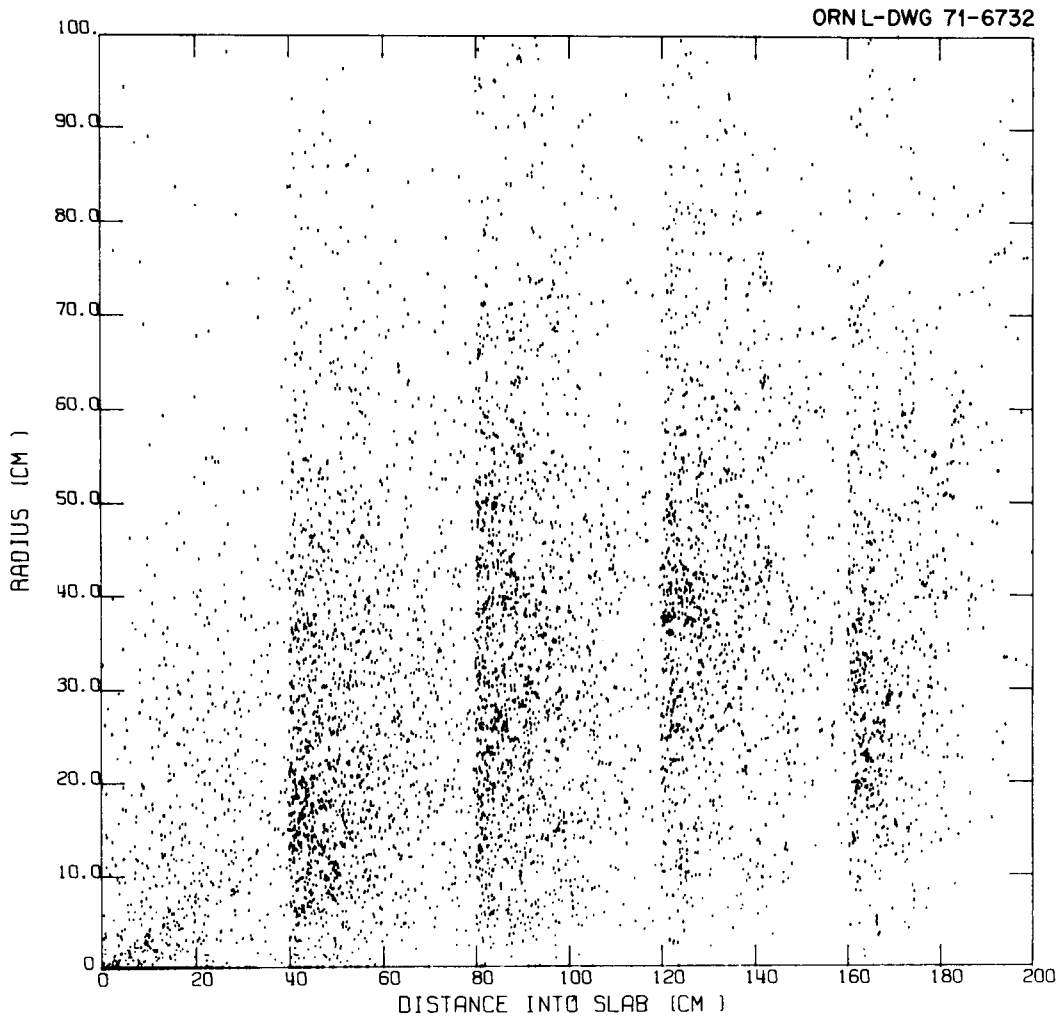

Fig. III-11. Distribution of Secondary Gamma-Ray Generations in Slab for 14-MeV Source Located at Origin (Importance Sampling Method III).

number of neutron histories. The number of secondary gamma-ray generations in Method III falls between Method I and II; however, the spatial distribution is different.

The Standard Method of biasing the secondary gamma-ray production produced nearly eight times as many gamma rays as did Method II. For the Standard Method 62% of the gamma rays were generated in the first two regions (first 80 cm), 33% in the next two regions (next 80 cm), and only 5% in the last region (last 40 cm). This distribution is similar to that for Method II which produced 53% of the gamma rays in the first two regions, 42% in the next two regions, and 5% in the last region.

For importance sampling Method III, 38% of the gamma-ray generations occurred in the first two regions, 45% in the next two regions, and 17% in the last region. The distribution of these gamma-ray generations as shown in Figure III-11 indicates that the gamma rays were produced in layers. This layering effect is due to the use of an insufficient number of spatial regions for averaging the weight standards $V_g(\bar{r})$. In order to evaluate the sensitivity of Method III to the number of averaging regions used, additional MORSE calculations* were performed in which the number of regions was increased from five to ten. The MORSE results showed a more uniform production of gamma rays across the slab with a corresponding change in the effect of interest from a value of 16% low (5 region) to only 5% low (10 region) when compared with the ANISN results. There was no significant change in the MORSE problem running

*In these calculations the effect of interest was the gamma-ray fluence in groups 23 to 32.

time with the increase in the number of regions. This would imply that an increase in the number of regions would improve the results for Method III. However, in order to obtain a valid comparison of these gamma-ray generation methods as presented in Table III-4 five regions were used in each of the calculations.

Distribution of Batch Estimates

Figures III-12, III-13, and III-14 show the distribution of the batch estimates of the gamma-ray dose at the shield surface about the mean compared with a normal distribution for Methods I, II, and III respectively (fission source case). Both the normal distribution (smooth curve) and the batch distribution (histogram) are normalized to a unit area under the curve. Each bin of the histogram represents a width of 25% of the batch standard deviation. The height of the histogram is then proportional to the fraction of the total of 40 batches that fell within a particular bin. For the normal distribution, the batch standard deviation represents the limits within which 68% of the batches should lie, i.e., if an additional batch estimate were made there would be a 68% probability of it falling within one batch standard deviation of the mean. It is obvious that the histogram does not approximate a normal distribution, but is skewed such that more than 50% of the total area falls below the mean. This is characteristic of deep-penetration shielding problems where the large percentage of the estimates which give a low answer are offset by a few rather large estimates which raise the mean value. However, the skewed distribution does indicate that more detailed biasing would be required in the Monte Carlo calculations

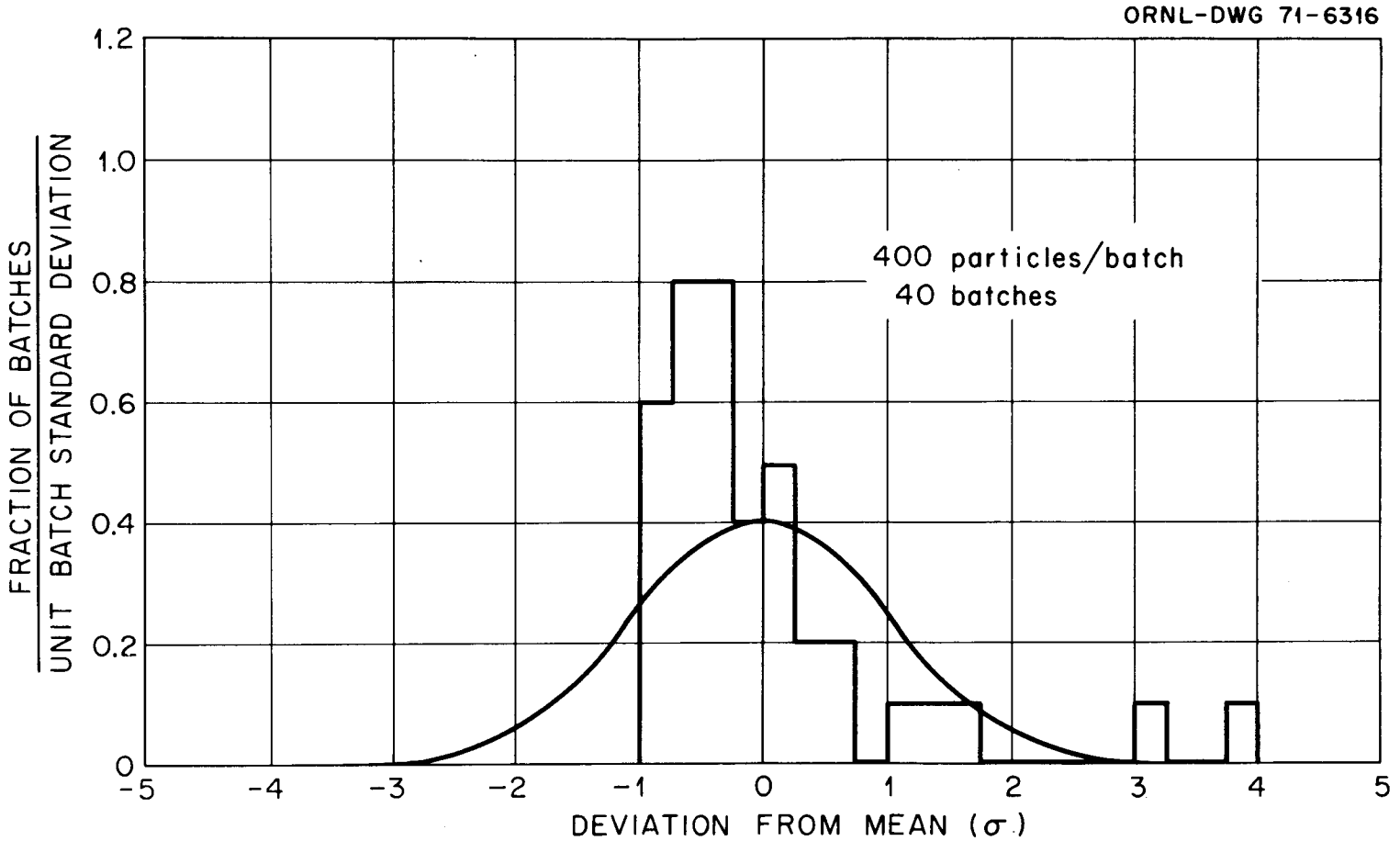

Fig. III-12. Comparison of Distribution of Batch Estimates of Gamma-Ray Dose at Shield Surface with a Normal Distribution. Fission Source Case - Importance Sampling Method I. (Fractional Batch Standard Deviation = 0.32)

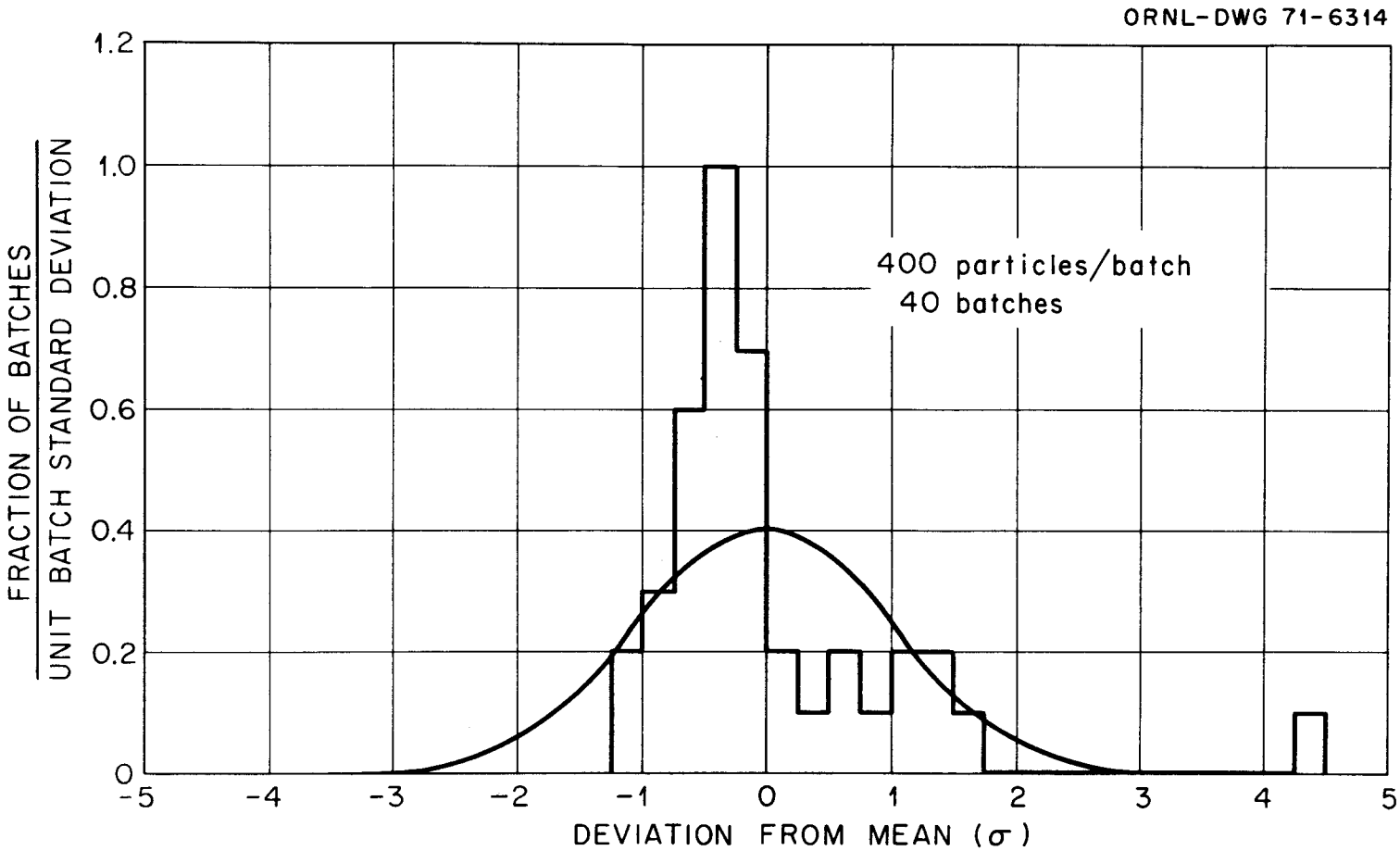

Fig. III-13. Comparison of Distribution of Batch Estimates of Gamma-Ray Dose at Shield Surface with a Normal Distribution. Fission Source Case - Importance Sampling Method II. (Fractional Batch Standard Deviation = 0.57)

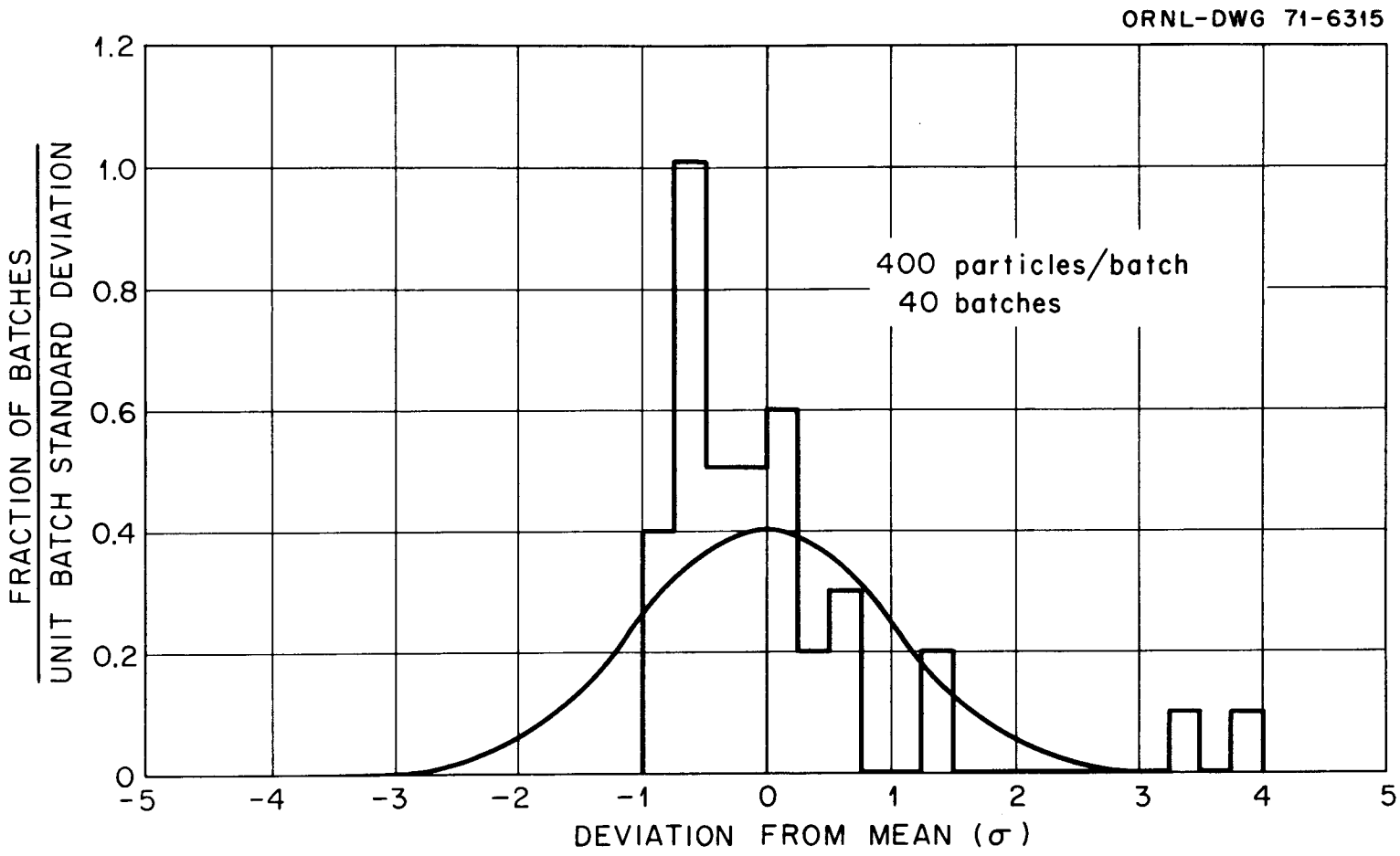

Fig. III-14. Comparison of Distribution of Batch Estimates of Gamma-Ray Dose at Shield Surface with a Normal Distribution. Fission Source Case - Importance Sampling Method III. (Fractional Batch Standard Deviation = 0.63)

to give a tighter distribution of the batch estimates. The histograms obtained from calculations using the three methods of gamma-ray biasing all exhibit this same general skewness.

The dose due to neutrons is not reported for the MORSE calculations since all of the biasing was done with the gamma-ray dose as the effect of interest and consequently the statistics on the neutron dose was very poor. However, the ANISN calculations showed the neutron dose to be a factor of 8 lower than the gamma-ray dose in the 14-MeV source case and a factor of 135 lower in the fission source case.

CHAPTER IV

CONCLUSION AND RECOMMENDATIONS

Three methods of biasing the production of secondary gamma rays in coupled, multigroup, Monte Carlo transport calculations have been developed. These methods employed important sampling techniques which include alteration of the gamma-ray generation probabilities, non-absorption weighting, and a combination of splitting and Russian roulette. The importance functions used for this importance sampling were obtained from a discrete ordinates solution to the adjoint Boltzmann equation.

The three biasing methods were evaluated in their application to deep-penetration Monte Carlo calculations in concrete for both a 14-MeV and a fission source. Method I was found to be the most efficient method of obtaining an answer for both source cases. However, all three methods were shown to be superior than the standard method of secondary gamma-ray generation used in the MØRSE code. The methods varied from a factor of 1.3 to 40.0 better than the standard method based on the running time of the code and the variance of the answer obtained.

It is felt that the results of these calculations demonstrate the applicability of these importance sampling methods in deep penetration, coupled, multigroup, Monte Carlo calculations and provide an evaluation of their effectiveness. However, before routinely utilizing these methods, further research into their application in deep penetration should perhaps be performed. This research might include investigation

in multi-media problem as well as problems in which the effect of interest includes both neutrons and gamma rays. Also investigation might be performed into the applicability of these methods to the coupled adjoint mode of the multigroup Monte Carlo calculations as well as to Monte Carlo calculations which employ point cross-section data.

The calculation of the importance function as an integral part of the Monte Carlo calculation might be investigated as a method of further increasing the efficiency of these importance sampling methods.

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APPENDIX A

The time-independent integro-differential form of the Boltzmann transport equation is given by

$$\bar{\Omega}\cdot\nabla\phi(\bar{r},E,\bar{\Omega}) + \Sigma_t(\bar{r},E)\ \phi(\bar{r},E,\bar{\Omega}) \tag{A-1}$$

$$= S(\bar{r},E,\bar{\Omega}) + \iint dE'\ d\Omega'\ \Sigma_s(\bar{r},E\leftarrow E',\bar{\Omega}\leftarrow\bar{\Omega}')\ \phi(\bar{r},E',\bar{\Omega}')$$

$(\bar{r},E,\bar{\Omega})$ = the six-dimensional phase space.

$\bar{r}$ = position variable.

E = the particles' kinetic energy.

$\bar{\Omega}$ = a unit vector which describes the particles' direction of motion,

$\phi(\bar{r},E,\bar{\Omega})$ = time-independent angular flux,

$\phi(\bar{r},E,\bar{\Omega})dEd\bar{\Omega}$ = the number of particles that cross a unit area normal to the $\bar{\Omega}$ direction per unit time at space point $\bar{r}$ with energies in dE about E and with directions that lie within the differential solid angle $d\bar{\Omega}$ about the unit vector $\bar{\Omega}$.

$\bar{\Omega}\cdot\nabla\phi(\bar{r},E,\bar{\Omega})dEd\bar{\Omega}$ = net convective loss per unit volume and time at the space point $\bar{r}$ of particles with energies in dE about E and direction which lie in $d\bar{\Omega}$ about $\bar{\Omega}$.

$\Sigma_t(r,E)$ = the total cross section at the space point $\bar{r}$ for particles of energy E,

$\Sigma_t(r,E)\phi(\bar{r},E,\bar{\Omega})dEd\bar{\Omega}$ = collision loss per unit volume and time at the space point $\bar{r}$ of particles with energies in dE about E and directions which lie in $d\bar{\Omega}$ about $\bar{\Omega}$.

$\Sigma_s(\bar{r},E\leftarrow E',\bar{\Omega}\leftarrow\bar{\Omega}')dEd\bar{\Omega}$ = the differential cross section which describes the probability per unit path that a particle with an initial energy E' and an initial direction $\bar{\Omega}'$ undergoes a collision at $\bar{r}$ which places it into a direction that lies in $d\bar{\Omega}$ about $\bar{\Omega}$ with a new energy in dE about E.

$\left[\iint \Sigma_s(\bar{r},E\leftarrow E',\bar{\Omega}\leftarrow\bar{\Omega}')\phi(\bar{r},E',\bar{\Omega}')dE'd\bar{\Omega}'\right] dEd\bar{\Omega}$ = the gain per unit volume and time at the space point $\bar{r}$ of particles with energies in dE about E and directions which lie in $d\bar{\Omega}$ about $\bar{\Omega}$.

$S(\bar{r},E,\bar{\Omega})dEd\bar{\Omega}$ = source particles emitted per unit volume and time at the space point $\bar{r}$ with energies in dE about E and directions which lie in $d\bar{\Omega}$ about $\bar{\Omega}$.

A group form of Eq. (A-1) is obtained by integrating each term with respect to the energy variables over the energy integral ΔEg where

ΔEg = energy width of the gth group,

g = 1 corresponds to the highest energy group,

g = N corresponds to the lowest energy group,

with the obvious constraint that

$$\sum_{g=1}^{N} \Delta Eg = \int_0^{E_o} dE = E_o, \text{ the maximum particle energy.}$$

The integration of each term over the gth energy group yields

$$\bar{\Omega}\cdot\nabla \int_{\Delta Eg} \phi(\bar{r},E,\bar{\Omega})dE + \int_{\Delta Eg} \Sigma_t(\bar{r},E)\phi(\bar{r},E,\bar{\Omega})dE \tag{A-2}$$

$$= \int_{\Delta Eg} S(\bar{r},E,\bar{\Omega})dE + \sum_{g'=g}^{1} \int_{\Delta Eg'}\int_{4\pi} dE'd\bar{\Omega}' \int_{\Delta Eg}$$

$$\times\ \Sigma_s(\bar{r},E\leftarrow E',\bar{\Omega}\leftarrow\bar{\Omega}')\phi(\bar{r},E',\bar{\Omega}')dE$$

Equation (A-2) provides the formal basis for the following group parameters:

$$\phi_g(\bar{r},\bar{\Omega}) = \text{time-independent group angular flux}$$

$$= \int_{\Delta Eg} \phi(\bar{r},E,\bar{\Omega})dE$$

$$\Sigma_t^g(\bar{r}) = \text{energy-averaged total cross section for the gth group}$$

$$= \frac{\int_{\Delta Eg} \Sigma_t(\bar{r},E)\phi(\bar{r},E,\bar{\Omega})dE}{\int_{\Delta Eg} \phi(\bar{r},E,\bar{\Omega})dE}$$

$$\Sigma_s^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}') = \text{group g'-to-group g transfer cross section}$$

$$= \frac{\int_{\Delta Eg'}\int_{\Delta Eg} \Sigma_s(\bar{r},E\leftarrow E',\bar{\Omega}\leftarrow\bar{\Omega}')\phi(\bar{r},E',\bar{\Omega}')dE'dE}{\int_{\Delta Eg'} \phi(\bar{r},E',\bar{\Omega}')dE'}$$

$$S_g(\bar{r},\bar{\Omega}) = \text{source particles for the gth group}$$

$$= \int_{\Delta Eg} S(\bar{r},E,\bar{\Omega})dE \quad .$$

Thus equation (A-2) may be written

$$\bar{\Omega}\cdot\nabla\phi_g(\bar{r},\bar{\Omega}) + \Sigma_t^g(\bar{r})\phi_g(\bar{r},\bar{\Omega}) = S(\bar{r},\bar{\Omega}) \tag{A-3}$$

$$+ \sum_{g'=g}^{1} \int d\bar{\Omega}' \; \Sigma_s^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}') \; \phi_{g'}(\bar{r},\bar{\Omega}')$$

where the summation over energy groups could be expanded over all g' to allow for upscatter of particles. This equation can be transformed into an integral form in terms of the emergent particle density $\chi_g(\bar{r},\bar{\Omega})$ where

$\chi_g(\bar{r},\bar{\Omega})d\bar{\Omega}$ = the expected number of particles leaving a source or emerging from a real collision per unit volume and time at the space point $\bar{r}$ in energy group g and directions which lie in $d\bar{\Omega}$ about $\bar{\Omega}$.

The emergent particle density is therefore given by

$$\chi_g(\bar{r},\bar{\Omega}) = S_g(\bar{r},\bar{\Omega}) + \sum_{g'=g}^{1} \int_{4\pi} d\bar{\Omega}'\Sigma_s^{g\leftarrow g'}(\bar{r},\bar{\Omega}\leftarrow\bar{\Omega}')\phi_{g'}(\bar{r},\bar{\Omega}') \tag{A-4}$$

which is simply the right hand side of equation (A-3).

Consequently $\chi_g(\bar{r},\bar{\Omega})$ must also be equal to the left hand side of equation (A-3)

$$\chi_g(\bar{r},\bar{\Omega}) = \bar{\Omega}\cdot\nabla\phi_g(\bar{r},\bar{\Omega}) + \Sigma_t^g(\bar{r})\phi_g(\bar{r},\bar{\Omega}) \quad . \tag{A-5}$$

In order to obtain a solution to the above equation, the convection term is expressed in terms of the spatial variable R which relates a fixed point in space $(\bar{r})$ to an arbitrary point $(\bar{r}')$ as shown in Figure A-1.

The total derivative of the group angular flux with respect to R is

$$\begin{aligned} \frac{d}{dR}\phi_g(\bar{r},\bar{\Omega}) &= \frac{\partial x}{\partial R}\frac{\partial\phi}{\partial x} + \frac{\partial y}{\partial R}\frac{\partial\phi}{\partial y} + \frac{\partial z}{\partial R}\frac{\partial\phi}{\partial z} \\ &= -\Omega_x\frac{\partial\phi}{\partial x} - \Omega_y\frac{\partial\phi}{\partial y} - \Omega_z\frac{\partial\phi}{\partial z} \\ &= \bar{\Omega}\cdot\nabla\phi_g(\bar{r},\bar{\Omega}) \quad . \end{aligned} \tag{A-6}$$

Using the relationship, equation (A-5) can be written at $\bar{r}'$ as

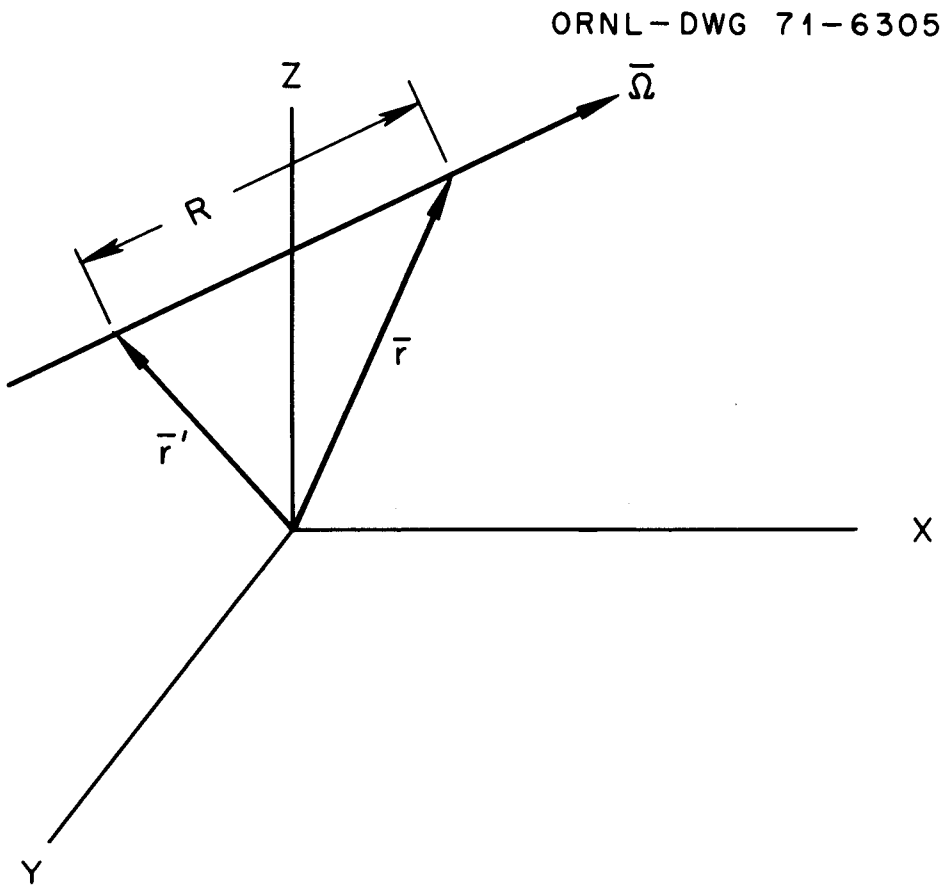

Fig. A-I. Coordinate System Which Relates a Fixed Point $\overline{r}$ to an Arbitrary Point $\overline{r}'$ in Terms of the Spatial Variable R: $\overline{r}' = \overline{r} - R\overline{\Omega}$.

$$- \frac{d}{dR} \phi_g(\bar{r}',\bar{\Omega}) + \Sigma_t^g(\bar{r}')\phi_g(\bar{r}',\bar{\Omega}) = \chi_g(\bar{r}',\bar{\Omega}) \quad . \tag{A-7}$$

To solve equation (A-7) for $\phi_g(\bar{r}',\bar{\Omega})$ we multiply by an integrating factor

$$e^{-\int_o^R \Sigma_t^g(\bar{r}-R'\bar{\Omega})dR'}$$

Then equation (A-7) can be written

$$- \frac{d}{dR} \left[\phi_g(\bar{r}',\bar{\Omega}) \; e^{-\int_o^R \Sigma_t^g(\bar{r}-R'\bar{\Omega})dR'} \right] \tag{A-8}$$

$$= \chi_g(\bar{r}',\bar{\Omega}) \; e^{-\int_o \Sigma_t^g(\bar{r}-R'\bar{\Omega})dR'} \quad .$$

Multiply equation (A-8) by dR and integrate (R = 0, R = ∞), then

$$\phi_g(r,\bar{\Omega}) - \phi_g(\infty,\bar{\Omega}) \; e^{-\int_o^\infty \Sigma_t^g(r-R'\Omega)dR'} \tag{A-9}$$

$$= \int_o^\infty \chi_g(\bar{r}',\bar{\Omega}) \; e^{-\int_o^R \Sigma_t^g(\bar{r}-R'\bar{\Omega})dR'} \; dR \quad .$$

Require that

$$\phi_g(\infty,\bar{\Omega}) \; e^{-\int_o^\infty \Sigma_t^g(\bar{r}-R'\bar{\Omega})dR'} = 0 \quad . \tag{A-10}$$

Thus the solution for $\phi_g(\bar{r},\bar{\Omega})$ is given by

$$\phi_g(\bar{r},\bar{\Omega}) = \int_0^\infty \chi_g(\bar{r}-R\bar{\Omega},\bar{\Omega})\, e^{-\int_0^R \Sigma_t^g(\bar{r}-R'\bar{\Omega})dR'}\, dR \qquad \text{(A-11)}$$

which gives the group g angular flux at $\bar{r}$ in direction $\bar{\Omega}$ in terms of the density of particles leaving collisions in group g at $\bar{r} - R\bar{\Omega}$ and in direction $\bar{\Omega}$.

In order to make this equation more general such that $\phi_g(\bar{r},\bar{\Omega})$ is given in terms of the density of particles leaving collision at any arbitrary angle $\bar{\Omega}'$ it is necessary to define a delta function $\delta(\bar{\Omega}',\bar{\Omega})$ with the properties that

$$\delta(\bar{\Omega}',\bar{\Omega}) = 0 \qquad \text{if } \bar{\Omega}' \neq \bar{\Omega}$$

and

$$\int^{\bar{\Omega}'} \delta(\bar{\Omega}',\bar{\Omega})d\bar{\Omega}' = 1 \quad .$$

Then equation (A-11) can be rewritten as

$$\phi_g(\bar{r},\bar{\Omega}) = \int^{\bar{\Omega}'} \delta(\bar{\Omega}',\bar{\Omega})d\bar{\Omega}' \qquad \text{(A-12)}$$

$$\times \int_0^\infty \chi_g(\bar{r}-R\bar{\Omega},\bar{\Omega})\, e^{-\int_0^\infty \Sigma_t^g(\bar{r}-R'\bar{\Omega})dR'}\, dR \quad .$$

Now with

$$d\bar{r}' = R^2 d\bar{\Omega}' dR$$

and

$$\int f(\overline{\Omega}')\ \delta(\overline{\Omega}',\overline{\Omega})d\overline{\Omega}' = f(\overline{\Omega}) \tag{A-13}$$

Equation (A-12) becomes

$$\phi_g(r,\overline{\Omega}) = \int^{\overline{r}'} \chi_g(\overline{r}-R\overline{\Omega}',\overline{\Omega}') \tag{A-14}$$

$$e^{-\int_o^R \Sigma_t^g(\overline{r}-R'\overline{\Omega}')dR'} \frac{\delta(\overline{\Omega}',\overline{\Omega})}{R^2}\, d\overline{r}'$$

which gives the group g angular flux at $\overline{r}$ in direction $\overline{\Omega}'$ in terms of the density of particles leaving collisions in group g at an arbitrary space point $\overline{r}'$ in an arbitrary direction $\overline{\Omega}'$.

This group angular flux may be substituted into equation (A-4) to give

$$\chi_g(\overline{r},\overline{\Omega}) = S_g(\overline{r},\overline{\Omega}) + \sum_{g'=g}^{1} \int^{\overline{r}'}\int^{4\pi} \Sigma_s^{g\leftarrow g'}(\overline{r},\overline{\Omega}\leftarrow\overline{\Omega}'') \tag{A-15}$$

$$\times\ e^{-\int_o^R \Sigma_t^g(\overline{r}-R'\overline{\Omega}')dR'} \frac{\delta(\overline{\Omega}',\overline{\Omega}'')}{R^2}\, \chi_{g'}(\overline{r}-R\overline{\Omega}',\overline{\Omega}')d\overline{\Omega}''d\overline{r}'$$

where the arbitrary angle of integration at space point $\overline{r}$ has been denoted $\overline{\Omega}''$ in order to distinguish it from $\overline{\Omega}'$ which is the angle of integration at $\overline{r}'$. Equation (A-15) then gives the density of particles leaving collisions in group g at $\overline{r}$ in direction $\overline{\Omega}$ in terms of the density of particles leaving collisions in group g' at $\overline{r}'$ in direction $\overline{\Omega}'$.

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