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SHIELD WEIGHT OPTIMIZATION USING MONTE CARLO TRANSPORT CALCULATIONS

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This report outlines the theory used in FASTER-III, a Monte Carlo computer program for the transport of neutrons and gamma rays in complex geometries. The code has the additional capability of calculating the minimum weight layered unit shield configuration which will meet a specified dose rate constraint. It includes the treatment of geometric regions bounded by quadratic and quadric surfaces with multiple radiation sources which have a specified space, angle, and energy dependence. The program calculates, using importance sampling, the resulting number and energy fluxes at specified point, surface, and volume detectors.

Results are presented for sample problems involving primary neutron and both primary and secondary photon transport in a spherical reactor-shield configuration. These results include the optimization of the shield configuration.

Section 1
INTRODUCTION AND SUMMARY

The original FASTER program (ref. 1) contained a number of new techniques which provided the capability of obtaining accurate radiation levels at specified points in complex geometries. Prior use of FASTER indicated a need to broaden the overall program capabilities, automate the importance sampling, increase the computational efficiency, and revise the users manual. This revised program has been designated FASTER-III to distinguish it from earlier versions.

A specific program capability permitting the calculation of minimum weight layered unit shield configurations for mobile nuclear reactor applications, e.g., nuclear propulsion for aircraft, surface effect vehicles, and spacecraft has recently been developed. The basic Monte Carlo transport method was extended to include a calculation of partial derivatives of the radiation fluxes with respect to specified shield dimensions. These derivatives are then used to define exponential relationships used in the shield optimization procedure. This optional program feature is described more completely in Section 2.

Data preparation is simple, with very little judgment required to set up the importance sampling for most problems. The code also has a unit shield weight optimization capability.

Particularly noteworthy features of FASTER-III are the following:

(1) A calculation of optimal importance sampling parameters based on partial derivatives of the variance (Section 2.3).

(2) The acceptance of data in either fixed or variable field formats including the ANISN-DTF format for neutron cross sections.

(3) The calculation of time-dependent neutron and photon transport (using time moments and/or time intervals) including an optional exponential atmosphere.

(4) The improvement and addition of importance sampling models with the various importance sampling parameters built into the program.

Various program features are described in Refs. 2 to 6.

The application of the FASTER-III program to a shield optimization problem is discussed in Section 3. The problem involved a spherical reactor-shield configuration and included primary neutrons and both primary and secondary photons. Conclusions and recommendations are presented in Section 4.

Section 2
ANALYSIS

The techniques used in calculating optimum shield configurations and optimum importance sampling parameters are summarized below. The discussion is given in three parts: dose rate derivatives with respect to shield layer thicknesses, optimization procedures, importance parameter optimization.

2.1 Dose Rate Derivatives

The dose rate at a point detector $\underline{y}$ for a specified reactor shield configuration is written as:

$$D(\underline{y}) = \sum_{j=1}^{J} R_j \varphi_j(\underline{y}) \qquad (1)$$

where J is the total number of energy groups for both neutrons and photons (including secondaries), $\varphi_j(\underline{y})$ is the particle flux in the jth energy group, and R_j is the response function to convert from flux to dose rate. The rate of change of the dose rate with respect to a shield layer thickness is simply

$$\frac{\partial D(\underline{y})}{\partial t_l} = \sum_{j=1}^{J} R_j \frac{\partial \varphi_j(\underline{y})}{\partial t_l} \qquad l = 1, 2, \ldots, L \qquad (2)$$

where L is the total number of shield layers and t_l is the thickness of the lth layer. The equation used by the program for determining the flux is written as:

$$\varphi_j(\underline{y}) = \frac{1}{N} \sum_{n=1}^{N} \sum_{k} S^*_{jkn}(\underline{u}_{kn}) K_j(\underline{z}_{kn}, \underline{y}),$$

$$\underline{u}_{kn} = \frac{\underline{y} - \underline{z}_{kn}}{|\underline{y} - \underline{z}_{kn}|} \quad (3)$$

where N is the total number of histories tracked via the Monte Carlo method, k is the number of particle collisions, $\underline{z}_{kn}$ is the position of the kth collision of the nth history, $S^*_{jkn}(\underline{u}_{kn})$ the number of particles in the jth energy group emerging from $\underline{z}_{kn}$ in the direction $\underline{u}_{kn}$ of the detector per unit solid angle, and $K_j(\underline{z}_{kn}, \underline{y})$ represents the material and geometric attenuation kernel for particles in the jth energy group going from $\underline{z}_{kn}$ to the detector.

The partial derivative of the flux with respect to the lth shield layer thickness is simply:

$$\frac{\partial \varphi_j(\underline{y})}{\partial t_l} = \frac{1}{N} \sum_{n=1}^{N} \sum_{k} \frac{\partial}{\partial t_l} \left[S^*_{jkn}(\underline{u}_{kn}) K_j(\underline{z}_{kn}, \underline{y}) \right] \quad (4)$$

The summations are a minor part of the calculation. Therefore, the notation is simplified by concentrating on the elements in the summation

$$\frac{\partial \theta_{jkn}}{\partial t_l} = \frac{\partial}{\partial t_l} \left[S^*_{jkn}(\underline{u}_{kn}) K_j(\underline{z}_{kn}, \underline{y}) \right] \quad (5)$$

where θ_{jkn} represents the contribution to the flux in the jth energy group from the kth collision of the nth history. This equation is rewritten as

$$\frac{\partial \theta_{jkn}}{\partial t_l} = \theta_{jkn} \frac{\partial}{\partial t_l} \ln \left[S^*_{jkn}(\underline{u}_{kn}) K_j(\underline{z}_{kn}, \underline{y}) \right]$$

$$= \theta_{jkn} \left[\frac{\partial}{\partial t_l} \ln S^*_{jkn}(\underline{u}_{kn}) + \frac{\partial}{\partial t_l} \ln K_j(\underline{z}_{kn}, \underline{y}) \right] \quad (6)$$

The second term in brackets involves the attenuation kernel

$$K_j(\underline{z}_{kn}, \underline{y}) = \frac{\exp\left[- \sum_{m=1}^{M} s_m \sigma_{jm} \right]}{s^2} \quad (7)$$

where M is the total number of regions traversed from $\underline{z}_{kn}$ to the detector, s_m is the path length for the mth region traversed, σ_{jm} is the total cross section of this region for particles in the jth energy group, and s is the total distance from $\underline{z}_{km}$ to the detector, i.e.,

$$s = \sum_{m=1}^{M} s_m \quad (8)$$

A substitution of this kernel gives:

$$\frac{\partial}{\partial t_l} \ln K_j(\underline{z}_{kn}, \underline{x}) = \frac{\partial}{\partial t_l} \left[- \sum_{m=1}^{M} s_m \sigma_{jm} - 2 \ln \sum_{m=1}^{M} s_m \right]$$

$$= - \sum_{m=1}^{M} \sigma_{jm} \frac{\partial s_m}{\partial t_l} - \frac{2 \sum_{m=1}^{M} \frac{\partial s_m}{\partial t_l}}{\sum_{m=1}^{M} s_m}$$

$$= - \sum_{m=1}^{M} \left(\sigma_{jm} + \frac{2}{s} \right) \frac{\partial s_m}{\partial t_l} \quad (9)$$

The partial derivative of the partial path length s_m with respect to the shield layer thickness t_l is zero unless the mth region traversed is affected by a change in t_l. In particular, if t_l is a characteristic dimension of the region, i.e., its thickness, then

$$\frac{\partial s_m}{\partial t_l} = \frac{1}{\mu_{knm}}, \quad \mu_{knm} = \underline{u}_{kn} \cdot \underline{n}_{knm} \quad (10)$$

where μ_{knm} is the cosine of the angle measured from the surface normal $\underline{n}_{knm}$, with which the particle crosses the boundary of the region.

In the strict sense, the change of the thickness of one shield region can affect other shield regions. In particular, for a spherically symmetric reactor-shield configuration, an increase in the thickness of a shield region forces a movement of all shield regions having a larger radius. The inclusion of these effects in the above equation unnecessarily complicates the analysis and the calculations. The primary effect of changing a shield region dimension is to change the number of mean free paths which particles have to traverse in reaching the detector. Therefore, in calculating the derivatives, only the effect of the material attenuation is treated.

The derivatives at a specific boundary crossing m' then simplify to:

$$\frac{\partial}{\partial t_l} \ln K_j(\underline{z}_{kn}, \underline{y}) = - \sum_{m=1}^{M} \left(\sigma_{jm} + \frac{2}{s} \right) \frac{\partial s_m}{\partial t_l}$$

$$= - \left(\sigma_{jm'} + \frac{2}{s} \right) \frac{1}{\mu_{knm'}} - \left(0 + \frac{2}{s} \right) \frac{1}{-\mu_{knm'}}$$

$$= - \sigma_{jm'} / \mu_{knm'} \quad (11)$$

where m' is the index of a region having t_l as a dimension. The partial derivatives of the particle weight with respect to the shield dimensions - the first term in brackets in Eq. (6) - are zero at the point of origin of all primary particles. For subsequent particle collisions, the derivatives are calculated using the relationship between particle weights on subsequent collisions:

$S^*_{jkn}(\underline{u}_{kn})$

$$= \frac{\sum_i S^*_{i,k-1,n}(\underline{v}_{kn}) K_i(\underline{z}_{k-1,n}, \underline{z}_{kn}) T_{ij}(\underline{z}_{kn}, \underline{v}_{kn} \cdot \underline{u}_{kn})}{p^*_{kn}(\underline{z}_{kn})}$$

$$\underline{v}_{kn} = \frac{\underline{z}_{kn} - \underline{z}_{k-1,n}}{|\underline{z}_{kn} - \underline{z}_{k-1,n}|} \tag{12}$$

where $S^*_{i,k-1,n}(\underline{v}_{kn})$ is the number of particles coming out of the previous collision point in the direction $\underline{v}_{kn}$ and in the $i\underline{th}$ energy group, $K_i(\underline{z}_{k-1,n}, \underline{z}_{kn})$ is the attenuation kernel between particle collision points, $T_{ij}(\underline{z}_{kn}, \underline{v}_{kn} \cdot \underline{u}_{kn})$ is the scattering kernel for transfer of particles from group i to group j, and $p^*_{kn}(\underline{z}_{kn})$ is the probability density function used in selecting the collision point.

A straightforward substitution gives

$$\frac{\partial}{\partial t_l} \ln S^*_{jkn}(\underline{u}_{kn}) = \frac{\partial}{\partial t_l} \ln \left[\frac{\sum_i S^*_{i,k-1,n}(\underline{v}_{kn}) K_i(\underline{z}_{k-1,n}, \underline{z}_{kn}) T_{ij}(\underline{z}_{kn}, \underline{v}_{kn} \cdot \underline{u}_{kn}}{p^*_{kn}(\underline{z}_{kn})} \right] \tag{13}$$

After some manipulation, this reduces to

$$\frac{\partial}{\partial t_l} \ln S^*_{jkn}(\underline{u}_{kn})$$

$$= \frac{1}{S^*_{jkn}(\underline{u}_{kn})} \sum_i V_{ijkn} \left[\frac{\partial}{\partial t_l} \ln S^*_{i,k-1,n}(\underline{v}_{kn}) \right.$$

$$\left. + \frac{\partial}{\partial t_l} \ln K_i(\underline{z}_{k-1,n}, \underline{z}_{kn}) - \frac{\partial}{\partial t_l} \ln p^*_{kn}(\underline{z}_{kn}) \right] \tag{14}$$

where

V_{ijkn}

$$= \frac{S^*_{i,k-1,n}(\underline{v}_{kn}) K_i(\underline{z}_{k-1,n}, \underline{z}_{kn}) T_{ij}(\underline{z}_{kn}, \underline{v}_{kn} \cdot \underline{u}_{kn})}{p^*_{kn}(\underline{z}_{kn})} \tag{15}$$

The first term in brackets in Eq. (14) is the same partial derivative for collision k-1 as the partial derivative now being calculated for collision k. Therefore, it is known, either identically zero for k=0, or as determined from Eq. (14) for $k > 0$. The second term in brackets in Eq. (14) is similar to the second term in brackets in Eq. (6) and is therefore determined by Eq. (11). The last term in brackets involves the definition of the probability density function used to select the collision point $\underline{z}_{kn}$.

The probability density function for a collision point has the form

$p^*_{kn}(\underline{z}_{kn})$

$$= q^*_{kn}(\underline{v}_{kn}) \frac{A(s)a(s) \exp\left[-\int_0^s a(s')ds'\right]}{\int_0^\infty A(s')a(s') \exp\left[-\int_0^{s'} a(s'')ds''\right]ds'} \tag{16}$$

where $q^*_{kn}(\underline{v}_{kn})$ is a probability density function used to select the particle direction, $s = |\underline{z}_{kn} - \underline{z}_{k-1,n}|$ is the distance of the selected collision point from the previous collision point, A(s) is an importance factor for each region which changes discontinuously at region boundaries, and a(s) is an effective cross section which changes discontinuously at region boundaries and which may change continuously within a region.

The derivative of the logarithm of $p^*_{kn}(\underline{z}_{kn})$ involves only those terms which change when a shield dimension changes, i.e.,

$$\frac{\partial}{\partial t_l} \ln p^*_{kn}(\underline{z}_{kn}) = \frac{\partial}{\partial t_l} \left[-\int_0^s a(s')ds' \right]$$

$$- \frac{\partial}{\partial t_l} \ln \left\{ \int_0^\infty A(s')a(s') \exp\left[-\int_0^{s'} a(s'')ds'' \right] ds' \right\} \tag{17}$$

Let s_l denote the distance to a boundary involving the $l\underline{th}$ shield dimension. If the first term on the left side of Eq. (17) is affected by a change in this shield dimension, i.e. if $s > s_l$, then

$$\frac{\partial}{\partial t_l} \left[-\int_0^s a(s')ds' \right] = -a(s_l) \frac{\partial s_l}{\partial t_l}$$

$$= -a(s_l) \frac{1}{\mu_{lkn}} \tag{18}$$

where $a(s_l)$ is the effective cross section at the boundary of the shield and μ_{lkn} is the cosine the particle path makes with the outer shield normal. If there is any crossing involving the $l\underline{th}$ shield dimension, the second term in Eq. (18) will always have a non-zero derivative, i.e.,

$$\frac{\partial}{\partial t_l} \ln \left\{ \int_0^\infty A(s')a(s') \exp\left[-\int_0^{s'} a(s'')ds''ds' \right] \right\}$$

$$= \frac{A(s_l)a(s_l) \frac{1}{\mu_{lkn}} \exp\left[-\int_0^{s_l} a(s')ds' \right]}{\left\{ \int_0^\infty A(s')a(s') \exp\left[-\int_0^{s'} a(s'')ds'' \right] ds' \right\}} \tag{19}$$

Curved shield surfaces may be crossed more than once along the path between two particle collision points. Therefore, a summation of Eqs. (18) and (19) over every intersection involving the lth shield dimension is required to completely evaluate Eq. (17).

2.2 Optimization Procedures

The shield optimization calculation yields the set of shield layer thicknesses $\underline{t}' = (t_1', t_2', \ldots, t_l', \ldots t_L')$ such that the dose rate, $D(\underline{t}')$, meets the dose constraint. The Monte Carlo calculation is performed for an initial set of shield layer thicknesses $\underline{t} = (t_1, t_2, \ldots t_l, \ldots, t_L)$ and yields a set of fluxes, $\varphi_j(\underline{t})$, $j = 1, 2, \ldots, J$ and derivatives, $\partial\varphi_j(t)/\partial t_l$, $j = 1, 2, \ldots, J$; $l = 1, 2, \ldots, L$. The assumption is made that the fluxes vary exponentially with respect to shield dimension changes in the form

$$\varphi_j(\underline{t}') = \varphi_j(\underline{t}) \exp\left[\underline{a}_j \cdot (\underline{t}' - \underline{t})\right] \qquad (20)$$

where $\underline{a}_j = (a_{j1}, a_{j2}, \ldots, a_{jL})$. It follows that

$$\frac{\partial\varphi_j(\underline{t})}{\partial t_l'} = \varphi_j(\underline{t}) \exp\left[\underline{a}_j \cdot (\underline{t}' - \underline{t})\right] \frac{\partial}{\partial t_l}\left[\underline{a}_j \cdot (\underline{t}' - \underline{t})\right]$$

$$= \varphi_j(\underline{t}')a_{jl} \qquad (21)$$

In particular

$$\frac{\partial\varphi_j(\underline{t})}{\partial t_l} = a_{jl}\varphi_j(\underline{t}) \qquad (22)$$

or

$$a_{jl} = \frac{\partial\varphi_j(\underline{t})}{\partial t_l} \Big/ \varphi_j(\underline{t}) \qquad (23)$$

The weight is also expressed as a function of the shield layer thicknesses. The weight is denoted by $W(t')$ and for spherically symmetric shields:

$$W(t') = \frac{4\pi}{3}\left\{\rho_1\left[(r_o + t_1')^3 - r_o^3\right] + \rho_2\left[(r_o + t_1' + t_2')^3 - (r_o + t_1')^3\right] + \ldots\right\}$$

$$= \frac{4\pi}{3}\sum_{l=1}^{L} \rho_l\left[\left(r_o + \sum_{m=1}^{l} t_m'\right)^3 - \left(r_o + \sum_{m=1}^{l-1} t_m'\right)^3\right] \qquad (24)$$

where ρ_l is the density of the lth shield region and r_o is the minimum shield radius.

The purpose of the optimization procedure is to minimize the weight $W(\underline{t}')$ subject to the dose rate constraint $D(\underline{t}') = D_o$ where D_o is a specified dose rate. At this optimum, a small weight perturbation in any layer causes the same dose rate change. The rate at which dose rate changes with respect to a shield weight change in the lth layer is given by

$$Q_l = \frac{\dfrac{\partial D(t')}{\partial t_l'}}{\dfrac{\partial W(\underline{t}')}{\partial t_l'}} = \text{constant}, \quad l = 1, 2, \ldots, L \qquad (25)$$

The necessary derivatives are:

$$\frac{\partial D(t')}{\partial t_l'} = \sum_{j=1}^{J} R_j \frac{\partial\varphi_j(\underline{t}')}{\partial t_l'} =$$

$$= \sum_{j=1}^{J} R_j a_{jl}\varphi_j(\underline{t}) \exp\left[\underline{a}_j \cdot (\underline{t}' - \underline{t})\right] \qquad (26)$$

and for spherically symmetric shield:

$$\frac{\partial W(\underline{t}')}{\partial t_l'} = 4\pi \sum_{i=l}^{L} \rho_j\left[\left(r_o + \sum_{m=1}^{i} t_m'\right)^2 - \left(r_o + \sum_{m=1}^{i-1} t_m'\right)^2\right] \qquad (27)$$

In arriving at the optimum shield, the total shield weight is built up in increments of weight ΔW. Each increment in shield weight is always associated with a particular shield layer thickness. At each iteration, the particular shield dimension is selected by examining the values of the shield weight quality factors, Q_l. Each factor Q_l represents the approximate change in dose rate per unit change in weight corresponding to a change in the lth shield dimension. Negative Q_l's are the most usual and correspond to shields for which an increase in weight - and shield dimensions - gives a decrease in dose rate. Positive Q_l's can occur, however, and correspond to shields for which an increase in weight also increases the dose rate.

If, at a particular iteration, the dose rate is above the dose rate constraint, the minimum shield weight increment would correspond to the least positive value of those Q_l's for which $Q_l > 0$ and for which $t_l' > t_l(\min)$, where $t_l(\min)$ is the minimum value of the lth shield layer thickness. If such a Q_l exists, the dose rate can be decreased while also decreasing the shield weight the maximum amount. If there isn't such a Q_l, the next best procedure is to find the most negative of the Q_l's for which $Q_l < 0$ and for which $t_l' < t_l(\max)$, where $t_l(\max)$ is the maximum value of the lth shield layer thickness. A change in that Q_l would give the maximum decrease in dose rate per unit increase in weight.

If the dose rate is below the specified dose rate at a particular iteration, the minimum shield weight increment would correspond to the least negative of those Q_l's for which $Q_l < 0$ and for which $t_l' > t_l(\min)$. If such a Q_l exists, the dose rate can be increased while decreasing the shield weight the maximum amount. If there isn't such a Q_l, the next best procedure is to find the most positive of those Q_l's for which $Q_l > 0$ and for which $t_l' < t_l(\max)$. A change in that Q_l would give the maximum increase in dose rate per unit increase in weight.

Assuming a particular value Q_m of the Q_l's is selected through the above arguments, the corresponding shield dimension t'_m is changed by a maximum amount Δt_m where Δt_m is calculated as

$$\Delta t_m = \frac{\Delta W}{\frac{\partial W(\underline{t}')}{\partial t'_m}} \tag{28}$$

If this change would put t'_m outside one of its specified limits, the value of t'_m would be set to that limit, i.e., $t_m(\min) \le t'_m \le t_m(\max)$. The shield weight increment ΔW is calculated as

$$\Delta W = \frac{D_o - D(\underline{t}')}{Q_m} \tag{29}$$

subject to the constraint that $|\Delta W| < \Delta W_o$ where ΔW_o is a specified maximum shield weight increment per iteration. Note that ΔW, and therefore Δt_m, may be positive or negative depending on the value of Q_m and whether the dose rate is above or below the dose rate constraint.

Once a shield layer thickness is changed, the dose, weight, and their derivatives are re-evaluated and the entire process is repeated. The optimization would be discontinued in several ways. If the dose rate equals the dose rate constraint within the relative error of the original Monte Carlo dose rate calculation, the program will proceed to the next problem - which may be identical except with more histories to tighten the convergence of Monte Carlo calculations. Similarly, if all shield layer thicknesses have reached their minimum or maximum values, and if the optimum shield cannot be determined with these constraints, the program would again proceed to the next problem. Finally, if the dose rate and dose rate constraint are decades apart in value, the program would reevaluate the fluxes and their derivatives by Monte Carlo every time the dose rate changed by more than a specified factor during the optimization procedure.

2.3 Importance Parameter Optimization

The optimization of the importance sampling must be performed for some function, e.g., dose rate, of the energy-dependent fluxes since there is a different optimum for every initial particle energy. Therefore, assume that a minimum variance calculation of the dose rate is required where

$$\bar{D}_N = \frac{1}{N}\sum_{n=1}^{N} D_n \tag{30}$$

where N is the total number of histories and D_n is the dose rate from the nth history and $\bar{D}_N$ is the average value of the dose rate after N histories. The relative error of this dose rate is given by

$$E_N = \frac{1}{\bar{D}_N}\left[\frac{1}{N^2}\left(\sum_{n=1}^{N} D_n^2 - N\bar{D}_N^2\right)\right] \tag{31}$$

Taking the logarithm of this equation and then performing a formal calculation of the partial derivative with respect to an unspecified parameter a yields

$$\begin{aligned}\frac{\partial}{\partial a}\ln E_N &= -\frac{\partial}{\partial a}\ln \bar{D}_N - \frac{\partial}{\partial a}\ln N \\ &+ \frac{1\partial}{2\partial a}\ln\left(\sum_{n=1}^{N} D_n^2 - N\bar{D}_N^2\right) = -\frac{\frac{\partial}{\partial a}\bar{D}_N}{\bar{D}_N} \\ &+ \frac{\sum_{n=1}^{N} D_n\frac{\partial D_n}{\partial a} - N\bar{D}_N^2\frac{\partial \bar{D}_N}{\partial a}}{\sum_{n=1}^{N} D_n^2 - N\bar{D}_N^2} \\ &= \frac{1}{N^2\bar{D}_N^3 E_N^2}\left[\bar{D}_N\sum_{n=1}^{N} D_n\frac{\partial D_n}{\partial a} - \left(\sum_{n=1}^{N} D_n^2\right)\frac{\partial \bar{D}_N}{\partial a}\right]\end{aligned} \tag{32}$$

Thus the partial derivative of the relative error with respect to the parameter a is:

$$\frac{\partial E_N}{\partial a} = \frac{1}{N^2\bar{D}_N^3 E_N}\left[\bar{D}_N\sum_{n=1}^{N} D_n\frac{\partial D_n}{\partial a} - \left(\sum_{n=1}^{N} D_n^2\right)\frac{\partial \bar{D}_N}{\partial a}\right] \tag{33}$$

The dose rate from the nth history is given by

$$D_n = \sum_{j=1}^{J} R_j \sum_{k} \varphi_{jkn} \tag{34}$$

where J is the total number of energy groups, k is the number of particle collisions, R_j is the flux to dose rate conversion factor for the jth energy group, and φ_{jkn} is the flux in the jth group from the kth collision of the nth history. Since

$$\frac{\partial \bar{D}_N}{\partial a} = \frac{1}{N}\sum_{i=1}^{n}\frac{\partial D_n}{\partial a}, \tag{35}$$

the calculations required to evaluate Eq. (33) all involve the summation of terms which involve

$$\frac{\partial D_n}{\partial a} = \frac{\partial}{\partial a}\sum_{j=1}^{J}\left(R_j\sum_{k}\varphi_{jkn}\right) = \sum_{j=1}^{J} R_j\sum_{k}\frac{\partial \varphi_{jkn}}{\partial a} \tag{36}$$

The remainder of the analysis, therefore, can be concentrated on the partial derivatives of the fluxes. All other operations which must be performed are given above.

The fluxes typically depend on the detector position $\underline{y}$, so the equation for the particle flux is written as

$$\varphi_{jkn}(\underline{y}) = S^*_{jkn}(\underline{u}_{kn})K_j(\underline{z}_{kn}, \underline{y}) \tag{37}$$

The transport kernel $K_j(\underline{z}_{kn}, \underline{y})$ does not involve any importance sampling parameters so that

$$\frac{\partial \varphi_{jkn}(\underline{y})}{\partial a} = \frac{\partial S^*_{jkn}(\underline{u}_{kn})K_j(\underline{z}_{kn}, \underline{y})}{\partial a} \tag{38}$$

This equation can also be written as

$$\frac{\partial \varphi_{jkn}(\underline{y})}{\partial a} = S^*_{jkn}(\underline{u}_{kn}) K_j(\underline{z}_{kn}, \underline{y}) \frac{\partial}{\partial a} \ln S^*_{jkn}(\underline{u}_{kn}) \quad (39)$$

Without going into great detail, it turns out that the particle weight $S^*_{jkn}(\underline{u}_{kn})$ is composed of a purely analytical numerator, $V_{jkn}(\underline{u}_{kn})$ and a denominator which is the product of all the probability density functions used to select the collision points, i.e.,

$$S^*_{jkn}(\underline{u}_{kn}) = \frac{V_{jkn}(\underline{u}_{kn})}{\prod_{l=0}^{k} p^*_{ln}(\underline{z}_{ln})} \quad (40)$$

Therefore,

$$\ln S^*_{jkn}(\underline{u}_{kn}) = \ln V_{jkn}(\underline{u}_{kn}) - \ln \prod_{l=0}^{k} p^*_{ln}(\underline{z}_{ln}) \quad (41)$$

Since $V_{jkn}(\underline{u}_{kn})$ does not explicitly involve any importance parameters, it follows that

$$\frac{\partial}{\partial a} \ln S^*_{jkn}(\underline{u}_{kn}) = - \frac{\partial}{\partial a} \ln \prod_{l=0}^{k} p^*_{ln}(\underline{z}_{ln})$$

$$= - \sum_{l=0}^{k} \frac{\partial}{\partial a} \ln p^*_{ln}(\underline{z}_{ln}) \quad (42)$$

Therefore, Eq. (39) can be re-written as

$$\frac{\partial \varphi_{jkn}(\underline{y})}{\partial a} = - \varphi_{jkn}(\underline{y}) \sum_{l=0}^{k} \frac{\partial}{\partial a} \ln p^*_{ln}(\underline{z}_{ln}) \quad (43)$$

Moreover, the partial derivatives are energy-independent so that Eq. (36) becomes

$$\frac{\partial D_n}{\partial a} = \sum_k \left(\sum_{j=1}^{J} R_j \varphi_{jkn}(\underline{y}) \right) \left(- \sum_{l=0}^{k} \frac{\partial}{\partial a} \ln p^*_{ln}(\underline{z}_{ln}) \right) \quad (44)$$

The evaluation of the partial derivatives of the probability density functions can be written as

$$\sum_{l=1}^{k} \frac{\partial}{\partial a} \ln p^*_{ln}(\underline{z}_{ln}) = \sum_{l=0}^{k-1} \frac{\partial}{\partial a} \ln p^*_{ln}(\underline{z}_{ln})$$

$$+ \frac{\partial}{\partial a} \ln p^*_{kn}(\underline{z}_{kn}) \quad (45)$$

At the kth collision, the first term on the left side of Eq. (45) is known, identically zero if $k = 0$. Therefore, the analysis is completed after examining the calculation of the second term.

At this point it is necessary to identify the particular importance parameter a. Since most of the importance sampling parameters have fairly involved roles, the technique will be applied here to a set of parameters which can have a reasonably simple role. These parameters consist of the relative importance I_r of each region. Normally these parameters are all equal. However, in asymmetric problems, it turns out that some regions are much more important in terms of their scattering contributions to a detector. Therefore, these important regions have a larger value of I_r.

The region importance enters into the selection of a collision point through the following probability density function:

$$p^*_{kn}(\underline{z}_{kn}) = \frac{I_r p^*_r(s)}{\sum_{h=1}^{H} I_h P^*_h} \quad (46)$$

where r is the region in which the collision occurs (selected at random), $p^*_r(s)$ is the piecewise continuous probability density function in this region at the selected collision point (a distance s from the previous collision point), H is the total number of regions in which the collision could have occurred, and P^*_h is the integral of $p^*_h(s')$ over the partial path length in region h.

Calculating the logarithm of each side of the equation yields:

$$\ln p^*_{kn}(\underline{z}_{kn}) = \ln I_r + \ln p^*_r(s) - \ln \sum_{h=1}^{H} I_h P^*_h \quad (47)$$

The partial derivative of Eq. (47) with respect to the specific importance parameter I_g - the relative importance of region g - yields

$$\frac{\partial}{\partial I_g} \ln p^*_{kn}(\underline{z}_{kn}) = \frac{1}{I_r} \delta_{gr} - \frac{\sum_{h=1}^{H} P^*_h \delta_{gh}}{\sum_{h=1}^{H} I_h P^*_h} \quad (48)$$

where $\delta_{gh} = 0$ if region h is not region g and $\delta_{gg} = 1$.

Thus Eq. (48) is evaluated during the random selection of the kth collision point and the final term necessary to evaluate Eq. (45) and all preceding equations has been determined.

The above analysis is used to calculate the partial derivatives of the relative error of the dose rate with respect to the relative importance I_r of each geometric region, and a similar analysis is performed for the other importance sampling parameters. The result of the complete Monte Carlo calculation is a set of partial derivatives which, for the region importance, are given by

$$\frac{\partial E_N}{\partial I_r} = \frac{1}{N^2 \bar{D}^3_N E_N} \left[\bar{D}_N \sum_{n=1}^{N} D_n \frac{\partial D_n}{\partial I_r} - \left(\sum_{n=1}^{N} D_n^2 \right) \frac{1}{N} \sum_{n=1}^{N} \frac{\partial D_n}{\partial I_r} \right] \quad (49)$$

where $\partial D_n / \partial I_r$ is obtained from Eq. (44) using Eqs. (45) and (48).

After the calculation is completed, optimal values of the importance sampling parameters are

calculated by requiring that the relative error be zero - not actually achieved of course.

By a first order expansion

$$E'_N = 0 = E_N + \sum_{z=1}^{R} \frac{\partial E_N}{\partial I_z} (I'_z - I_z) \qquad (50)$$

where R is the total number of regions. A simple gradient analysis says that $I'_z - I_z$ should be proportional to $\partial E_N/\partial I_z$ so that

$$I'_z = I_z + C \frac{\partial E_N}{\partial I_z} \qquad (51)$$

where, by substitution into Eq. (50),

$$C = \frac{-E_N}{\sum_{z=1}^{R} \left(\frac{\partial E_N}{\partial I_z}\right)^2} \qquad (52)$$

where z is a general phase space coordinate

The program prints the optimum values of I'_z and other importance parameters after completing the Monte Carlo flux calculation. This analysis is performed for every response function. After more experience is obtained with the technique, the program could be modified to change these parameters internally corresponding to a specified response function.

Section 3

SAMPLE PROBLEM RESULTS

Two problems were investigated using the shield optimization capabilities of the FASTER-III program. Both problems involved a spherical reactor-shield configuration and included primary neutrons and both primary and secondary photons.

The two problems were similar except for the power level, 375 MW and 600 MW respectively. Both problems used a flat radial distribution for the primary neutron and photon source distribution. The primary photon source included an infinite operation equilibrium fission product term.

The core radii for the two problems were 82.38 and 96.38 cm respectively, corresponding to a power density of 4.53 MW/ft^3. Following the core was a 7.62 cm Be reflector; a 5 cm depleted uranium shield; three depleted uranium-borated water shield layers of 57, 15, and 15 cm thickness and 6.4, 4.6, and 2.8 gm/cm^3 density respectively; and a 117 cm borated water shield. This base line shield configuration was based on parameters obtained from SANE-SAGE calculations and subsequent calculations using the UNAMIT program, Ref. 7. The reactor-shield compositions are given in Table 1.

The primary neutron transport calculation utilized multigroup cross sections for 26 energy groups. Fifteen energy groups were utilized for both primary and secondary photons. The secondary production cross sections included both inelastic and capture gammas.

These initial configurations were each analyzed for a point detector 30 ft from the core center by following approximately 500 energy-dependent packets of primary neutrons and photons and approximately 7000 packets of secondary photons. The dose rates obtained from these calculations are tabulated in Table 2 including a breakdown by secondary source region. Each of these problems required about 28 minutes on the UNIVAC 1108 computer.

The basic calculated dose rates and dose rate derivatives were also used by the FASTER-III program to calculate the minimum weight shield configuration which would give a dose rate of 0.25 mr/hr at the specified detector point. The final shield configurations following the optimization are given in Table 3.

In both cases, the optimum shield configuration is significantly different from the base line configuration. Since the base line configuration was not generated by the FASTER-III program it is difficult to discuss many factors entering into that calculation which would account for the different optimal configuration. It is noted, however, that the base line configuration was generated using parameters corresponding to a calculated dose rate an order of magnitude below the specified dose rate constraint, Ref. 8. As such, the base line configuration used in the FASTER-III program was determined from an extrapolation of a different base line configuration.

A more critical critique can be made of the FASTER-III results independently. First it is noted that neither problem saw a significant contribution, less than a few percent, from photon sources in the core region. In fact, the 600 MW reactor dose rate from this source was about a factor of two less than it was for the 375 MW reactor. This difference is ascribed to the problem statistics since core photon sources see approximately 30 mean free paths of shield material. Therefore, it is doubtful if this dose rate component is converged within a factor of two after only 500 packets but this does not introduce a significant error since the original contribution was only two percent of the total dose rate.

The small contribution from core photon sources decreases the amount of high Z shields required around the core. Therefore, both problems gave a significant change in the first two shield dimensions during the optimization. In the 375 MW problem, the first mixture of depleted uranium-borated water (ρ = 6.4 gm/cm^3) was eliminated entirely. In the 600 MW problem, the depleted uranium and most of the first mixture were eliminated.

The main difference between the two FASTER-III calculations was the shift in the placement of lighter shield mixes towards the core for the 600 MW problem. An examination of the secondary photon dose components indicates that the contribution from the outer two shields was about 25 percent for the 375 MW reactor and almost 50 percent for the 600 MW reactor. Since these sources depend on the neutron attenuation through the closer regions and since lower effective Z materials are better neutron attenuators on a weight basis, the 600 MW problem tends to replace high effective Z material with a lower effective Z material.

The differences in the contribution from secondary sources in the outer shield regions is greater than expected for the nominal difference in the core region. Therefore, much of the difference in these sources must be ascribed to statistical variations. In fact, both problems had approximately 25 to 30 percent calculated relative error in the total photon dose rate. It should be noted that the FASTER-III program includes a number of importance sampling techniques which could be used to decrease this error. However, both

problems were run using the built-in definitions of importance parameters. Alternatively, more histories could have been used although the computer time requirements would have become excessive.

Section 4
CONCLUSIONS AND RECOMMENDATIONS

The FASTER-III program was developed to calculate neutron and photon fluxes at specified points in complex geometries. Alternatively, it can also calculate fluxes averaged over specified surfaces and volumes. The program was designed such that data preparation is simple and so that very little judgment is required to set up the importance sampling for most problems. The FASTER-III program satisfies these requirements very well.

The shield weight optimization capability included in the FASTER-III program permits the calculation of both base line radiation levels and optimal shield thicknesses all in a single computer run. However, the very large attenuation factors involved in the domonstration problems yielded some questionable results. In particular, the statistical differences in the relative contribution from various secondary source regions caused corresponding variations in the relative distributions of shield materials. Of course the statistical variations would be less in problems with less overall attenuation.

The effect of statistical differences on the shield optimization can be reduced by following more packets. However, the computer times start to get excessive if this is the only approach used. It would be more fruitful in terms of the routine application of the program to expend some effort towards altering the importance sampling.

The FASTER-III program has the capability of calculating optimal importance parameters based on partial derivatives of the variance. This feature can be used in determining better importance sampling parameters for shield optimization problems. In fact, the overall program efficiency could be improved if this feature was utilized on a wide variety of problems with the results being used to improve the built-in importance sampling models and parameters.

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TABLE 1

SPHERICAL REACTOR-SHIELD CONFIGURATION

Element	Compositions (10^{24} atoms/cm^3)						
	CORE	REFLECTOR	U^{238} SHIELD	MIX 1 SHIELD	MIX 2 SHIELD	MIX 3 SHIELD	H_2O+B SHIELD
H	0.01976	0.0	0.0	0.0451	0.0516	0.0580	0.0645
Be^9	0.0	0.120	0.0	0.0	0.0	0.0	0.0337
B	0.0	0.0	0.0	0.000671	0.000766	0.000862	0.000958
O	0.01184	0.0	0.0	0.0226	0.0258	0.0290	0.0
Al	0.0512	0.0	0.0	0.0	0.0	0.0	0.0
Zr	0.01744	0.0	0.0	0.0	0.0	0.0	0.0
U^{235}	0.000979	0.0	0.0	0.0	0.0	0.0	0.0
U^{238}	0.000078	0.0	0.0482	0.01446	0.00964	0.00482	0.0

TABLE 2

RESULTS OF FASTER-III BASE LINE CALCULATIONS OF REACTOR SHIELD CONFIGURATIONS AT 30 FEET FROM CORE CENTER

DOSE RATE COMPONENT	DOSE RATE CONTRIBUTIONS AT 30 FEET FROM CORE CENTER	
	375 MW REACTOR (mr/hr)	600 MW REACTOR (mr/hr)
Photon Source Region		
Core	0.009	0.004
Reflector	3.5×10^{-6}	6.3×10^{-6}
Depleted Uranium	3.2×10^{-5}	1.3×10^{-5}
Mix 1 Shield	0.018	0.026
Mix 2 Shield	0.062	0.075
Mix 3 Shield	0.017	0.063
Borated Water Shield	0.011	0.022
Total Photons	0.120 ± 0.034	0.187 ± 0.054
Neutrons	0.020 ± 0.002	0.027 ± 0.003
Total	0.140	0.214

TABLE 3

RESULTS OF FASTER-III SHIELD OPTIMIZATION
(0.25 mr/hr at 30 feet)

Quantity	375 MW REACTOR		600 MW REACTOR	
	Initial	Final	Initial	Final
Dose Rate (mr/hr)				
Photon	0.120	0.126	0.187	0.153
Neutron	0.020	0.124	0.027	0.097
Total	0.140	0.250	0.214	0.250
Shield Weight (10^3kg)				
Depleted U	10.2	12.6	13.8	0.0
Mix 1	71.2	0.0	89.2	6.6
Mix 2	22.1	52.4	26.4	52.4
Mix 3	16.1	12.2	19.0	63.1
Water	86.7	80.3	97.7	85.3
Total	206.3	157.5	246.1	207.4
Shield Thickness (cm)				
Depleted U	5.0	6.1	5.0	0.0
Mix 1	57.0	0.0	57.0	7.0
Mix 2	15.0	57.3	15.0	48.4
Mix 3	15.0	13.5	15.0	51.4
Water	117.0	120.8	117.0	98.4