# NASA TECHNICAL NOTE

NASA TN D-7093

# SHIELDING APPLICATION OF PERTURBATION THEORY TO DETERMINE CHANGES IN NEUTRON AND GAMMA DOSES DUE TO CHANGES IN SHIELD LAYERS

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| 1. Report No. NASA TN D-7093 | 2. Government Accession No. | 3. Recipien |
|---|---|---|
| 4. Title and Subtitle SHIELDING APPLICATION OF PERTURBATION THEORY TO DETERMINE CHANGES IN NEUTRON AND GAMMA DOSES DUE TO CHANGES IN SHIELD LAYERS | | 5. Report Date November 1972 |
| | | 6. Performing Organization Code |
| 7. Author(s) Daniel Fieno | | 8. Performing Organization Report No. E-7070 |
| | | 10. Work Unit No. 503-05 |
| 9. Performing Organization Name and Address Lewis Research Center National Aeronautics and Space Administration Cleveland, Ohio 44135 | | 11. Contract or Grant No. |
| | | 13. Type of Report and Period Covered Technical Note |
| 12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D.C. 20546 | | |
| | | 14. Sponsoring Agency Code |

15. Supplementary Notes

16. Abstract

Perturbation theory formulas were derived and applied to determine changes in neutron and gamma-ray doses due to changes in various radiation shield layers for fixed sources. For a given source and detector position, the perturbation method enables dose derivatives with respect to density, or equivalently thickness, for every layer to be determined from one forward and one inhomogeneous adjoint calculation. A direct determination without the perturbation approach would require two forward calculations to evaluate the dose derivative due to a change in a single layer. Hence, the perturbation method for obtaining dose derivatives requires fewer computations for design studies of multilayer shields. For an illustrative problem, a comparison was made of the fractional change in the dose per unit change in the thickness of each shield layer in a two-layer spherical configuration as calculated by perturbation theory and by successive direct calculations; excellent agreement was obtained between the two methods.

| 17. Key Words (Suggested by Author(s)) Perturbation theory Shielding methods | 18. Distribution Statement Unclassified - unlimited | | |
|---|---|---|---|
| 19. Security Classif. (of this report) Unclassified | 20. Security Classif. (of this page) Unclassified | 21. No. of Pages 43 | 22. Price* $3.00 |

*For sale by the National Technical Information Service, Springfield, Virginia 22151

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# SHIELDING APPLICATION OF PERTURBATION THEORY TO DETERMINE CHANGES IN NEUTRON AND GAMMA DOSES DUE TO CHANGES IN SHIELD LAYERS

## by Daniel Fieno

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## SUMMARY

Perturbation theory formulas were derived and applied to determine changes in neutron and gamma-ray doses due to changes in various radiation shield layers for fixed sources. For a given source and detector position the perturbation method enables dose derivatives due to all layer changes to be determined from one forward and one inhomogeneous adjoint calculation. Hence, the perturbation method for obtaining dose derivatives requires fewer computations for design studies of multilayer shields.

An illustrative problem is presented in which a comparison was made of the fractional change in the detector dose per unit change in the thickness of each shield layer as calculated by perturbation theory and by successive direct calculation. The problem involved a neutron source surrounded by spherical layers of tungsten and lithium hydride. The perturbation theory gave $-0.238$ cm$^{-1}$ for the fractional change in the neutron dose per unit change in the tungsten layer thickness; the result from direct calculations was $-0.234$ cm$^{-1}$. Similar close agreement was obtained for the effect of a change in the thickness of the lithium hydride layer on the neutron dose and for the effects of changes in both the tungsten and lithium hydride layers on the detector dose due to secondary gamma rays generated in the tungsten layer.

## INTRODUCTION

Nuclear reactors for space propulsion systems or auxiliary power systems require shielding to protect personnel, system components, and/or payload from neutrons and gamma-ray radiation. These shields are usually composed of alternate layers of heavy metal and hydrogeneous material. One shielding problem for these systems is to determine the number, arrangement, and thickness of these shield layers that will result in minimum-weight shields while maintaining the radiation field at various positions around the system within prescribed limits.

One-dimensional shield weight optimization procedures have been evolved for the design of layered configurations (refs. 1 to 3) and these have been extended to constraints in several directions around two-dimensional configurations (refs. 3 to 5). All these require the determination of the change in dose at a detector due to a change in thickness of each layer of a given shield configuration. These are generally obtained with $S_n$ transport calculations, requiring at least as many separate calculations as there are shield layers. As the optimization proceeds and the configuration changes, this procedure has to be repeated until the configuration converges to an optimum one. The optimization procedure becomes time consuming and, particularly for two-dimensional configurations, would require excessive amounts of computer time.

The present work applies perturbation theory for systems with fixed sources to obtain information to apply to multilayer-shielding problems. The use of perturbation theory in reactor physics applications is not new (ref. 6), the primary usage being the determination of reactivity effects. The application of perturbation methods to nonreactivity problems appears mainly in the Russian literature (refs. 7 and 8). The perturbation method utilizes only one forward and one inhomogeneous adjoint solution for an initially selected layered shield configuration to determine all necessary dose derivatives at a detector for a given neutron or gamma-ray source component. The method appreciably reduces the amount of calculations required for multilayer shields. In addition, perturbation theory yields a considerable amount of other information concerning the effects of individual reaction processes (scattering, absorption, etc.) on the dose rate.

The equations for this shield perturbation method are developed in the appendix and are applied to a simple spherical system to determine the dose derivatives of the various layers with respect to the layer thickness. This illustrative problem also serves to demonstrate the ability of the perturbation method to extract additional informative data concerning interaction processes of the various shield materials.

## METHOD OF ANALYSIS

This section presents the equations used in the perturbation analysis for systems with fixed sources. The theory is outlined for a fixed-source neutron system since the results for fixed-source gamma systems and coupled neutron-gamma systems are similar in form. A more complete derivation of the equations is given in the appendix. The symbols used are mainly conventional; those that are not are defined.

Consider the time-independent multigroup form of the inhomogeneous neutron transport equation. This equation is given by

$$\vec{\Omega} \cdot \vec{\nabla}\phi_g(\vec{r}, \vec{\Omega}) + \sigma_g(\vec{r})\phi_g(\vec{r}, \vec{\Omega}) = Q_g(\vec{r}, \vec{\Omega})$$

$$+ \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sum_{g'} \sigma^l(\vec{r}, g' \to g) \cdot \sum_{m=-l}^{l} \phi_{l,m}^{g'}(\vec{r}) P_{l,m}(\vec{\Omega}) \qquad g = 1, 2, \ldots, G \qquad (1)$$

where $\phi_g(\vec{r}, \vec{\Omega})$ is the angular flux for group g, $\sigma_g$ is the macroscopic total cross section for group g, $Q_g(\vec{r}, \vec{\Omega})$ is the angular fixed source for group g, $\sigma^l(g' \to g)$ is the $l^{th}$-order expansion coefficient of the scattering from group g' to group g, $\phi_{l,m}^{g}(\vec{r})$ is the $(l, m)^{th}$ expansion coefficient of the angular flux for group g in a spherical harmonics series, and $P_{l,m}(\vec{\Omega})$ is the $(l, m)^{th}$ spherical harmonic as a function of the unit direction vector $\vec{\Omega}$. The boundary condition for the angular flux at the convex boundary of the system is taken as

$$\phi_g(\vec{r}_s, \vec{\Omega}^-) = 0 \qquad g = 1, 2, \ldots, G \qquad (2)$$

This boundary condition is the usual condition and implies that no neutrons enter the system from the vacuum. Here $\vec{r}_s$ indicates the outer boundary of the system and $\vec{\Omega}^-$ designates an inward direction.

Once the solution, $\phi_g(\vec{r}, \vec{\Omega})$, to equation (1) has been obtained, then a physical process which depends linearly on the angular flux may be written as a functional, F. The general multigroup form of F is given by

$$F = \sum_g \int_{\vec{\Omega}} \int_R \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) \, d\vec{r} d\Omega \qquad (3)$$

The functional F gives contributions caused by an interaction process for the neutrons in the system. The quantity $P_g(\vec{r}, \vec{\Omega})$ has the role of an interaction cross section for group g at position $\vec{r}$ for neutrons moving in the direction $\vec{\Omega}$. The integrations are over all directions and over the entire system designated by R.

If a functional at some specific point, $\vec{r}_d$, is required, equation (3) may be written as

$$F(\vec{r}_d) = \sum_g \int_{\vec{\Omega}} \int_R \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) \delta(\vec{r} - \vec{r}_d) \, d\vec{r} d\Omega \qquad (4a)$$

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$$F(\vec{r}_d) = \sum_g \int_{\vec{\Omega}} \phi_g(\vec{r}_d, \vec{\Omega}) P_g(\vec{r}_d, \vec{\Omega}) \, d\Omega \qquad (4b)$$

where $\delta(\vec{r} - \vec{r}_d)$ is the Dirac delta function. The general expression, equation (3), will be used in subsequent derivations. Equation (4a) will be invoked when results such as radiation dose at a given position are required.

Following Usachev (ref. 7) an equation can be derived for the importance of neutrons for the physical process described by the functional F. The importance $\psi_g(\vec{r}, \vec{\Omega})$, which is equal to the effect F at some detector position or region due to a unit source of neutrons placed in group g at $(\vec{r}, \vec{\Omega})$, is given in multigroup form by

$$-\vec{\Omega} \cdot \vec{\nabla} \psi_g(\vec{r}, \vec{\Omega}) + \sigma_g(\vec{r})\psi_g(\vec{r}, \vec{\Omega}) = P_g(\vec{r}, \vec{\Omega})$$

$$+ \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \cdot \sum_{g'} \sigma^l(\vec{r}, g \to g') \cdot \sum_{m=-l}^{l} \psi_{l,m}^{g'}(\vec{r}) P_{l,m}(\vec{\Omega}) \qquad g = 1, 2, \ldots, G \qquad (5)$$

The boundary condition for the importance $\psi_g(\vec{r}, \vec{\Omega})$ follows from the fact that, if a neutron escapes from the system, it cannot contribute to the physical process of interest. Therefore, its importance must be zero and the boundary condition becomes

$$\psi_g(\vec{r}_s, \vec{\Omega}^+) = 0 \qquad g = 1, 2, \ldots, G \qquad (6)$$

where $\vec{\Omega}^+$ designates an outward direction.

The next step in the analysis is to derive an equation in terms of a perturbation in the density of the material constituents of the system. The perturbation in the density of a material, which can be related to a change in the thickness of that material shielding layer, is introduced in the equations through the macroscopic cross sections and appears as a perturbation in the cross sections of the system. If equation (1) were solved directly with the perturbed cross sections, a perturbed value $\mathscr{F}_g(\vec{r}, \vec{\Omega})$ for the angular flux would be obtained. The transport equation for the perturbed system is

$$\vec{\Omega} \cdot \vec{\nabla} \mathscr{F}_g(\vec{r}, \vec{\Omega}) + \left[\sigma_g(\vec{r}) + \delta\sigma_g(\vec{r})\right] \mathscr{F}_g(\vec{r}, \vec{\Omega}) = Q_g(\vec{r}, \vec{\Omega}) + \delta Q_g(\vec{r}, \vec{\Omega})$$

$$+ \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \cdot \sum_{g'} \left[\sigma^l(\vec{r}, g' \to g) + \delta\sigma^l(\vec{r}, g' \to g)\right] \cdot \sum_{m=-l}^{l} \mathscr{F}_{l,m}^{g'}(\vec{r}) P_{l,m}(\vec{\Omega}) \qquad g = 1, 2, \ldots, G \quad (7)$$

along with the boundary condition

$$\mathscr{F}_g(\vec{r}_s, \vec{\Omega}^-) = 0 \qquad g = 1, 2, \ldots, G \tag{8}$$

In the preceding equation, $\mathscr{F}_g(\vec{r}, \vec{\Omega})$ represents the perturbed value of the angular flux for group g. Perturbations in the cross sections are indicated by $\delta\sigma$. To generalize the analysis, the source term $Q_g(\vec{r}, \vec{\Omega})$ is assumed to be perturbed by $\delta Q_g(\vec{r}, \vec{\Omega})$.

The neutron transport equation for the perturbed system (eq. (7)), along with the equation for the importance (eq. (5)) and the boundary condition (eqs. (6) and (8)), can be manipulated algebraically to give the following result:

$$\sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \delta\sigma_g(\vec{r})\psi_g(\vec{r}, \vec{\Omega})\mathscr{F}_g(\vec{r}, \vec{\Omega})$$

$$-\sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sum_{m=-l}^{l} \int_R d\vec{r} \sum_{g'} \mathscr{F}_{l,m}^{g'}(\vec{r}) \cdot \sum_g \delta\sigma^l(\vec{r}, g' \to g)\psi_{l,m}^{g}(\vec{r})$$

$$-\sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \psi_g(\vec{r}, \vec{\Omega})Q_g(\vec{r}, \vec{\Omega}) - \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \psi_g(\vec{r}, \vec{\Omega})\delta Q_g(\vec{r}, \vec{\Omega})$$

$$+\sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \mathscr{F}_g(\vec{r}, \vec{\Omega})P_g(\vec{r}, \vec{\Omega}) = 0 \tag{9}$$

Equation (9) is an exact relationship and represents a condition which the perturbed angular flux and importance must satisfy. If all the perturbations in equation (9) are zero, then equation (9) along with equation (3) gives the important result

$$F = \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \phi_g(\vec{r}, \vec{\Omega})P_g(\vec{r}, \vec{\Omega})$$

$$= \sum_g \int_{\vec{\Omega}} d\Omega \int d\vec{r}\, \psi_g(\vec{r}, \vec{\Omega})Q_g(\vec{r}, \vec{\Omega}) \tag{10}$$

The perturbed flux $\mathscr{F}_g(\vec{r}, \vec{\Omega})$ has been replaced by its unperturbed value $\phi_g(\vec{r}, \vec{\Omega})$. The result expressed by equations (3) and (10) is well known (ref. 9) and is a necessary condition which the angular fluxes and importances must satisfy.

In the perturbed system the functional $F^p$ for the physical process of interest is equal to

$$F^p = \sum_g \int_{\vec{\Omega}} \int_R \mathscr{F}_g(\vec{r}, \vec{\Omega}) P_g^p(\vec{r}, \vec{\Omega}) \, d\vec{r} \, d\Omega \tag{11}$$

Here the general case of a perturbed system is considered for which $P_g^p(\vec{r}, \vec{\Omega})$ is the perturbed value of the quantity $P_g(\vec{r}, \vec{\Omega})$. The quantity $P_g^p(\vec{r}, \vec{\Omega})$ is taken to be

$$P_g^p(\vec{r}, \vec{\Omega}) = P_g(\vec{r}, \vec{\Omega}) + \delta P_g(\vec{r}, \vec{\Omega}) \tag{12}$$

Next consider the difference $\delta F$ of the functionals $F^p$ and $F$. Using equations (10), (11), and (12) in equation (9) results in

$$\delta F = F^p - F$$

$$= - \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r} \, \delta\sigma_g(\vec{r}) \psi_g(\vec{r}, \vec{\Omega}) \mathscr{F}_g(\vec{r}, \vec{\Omega})$$

$$+ \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \sum_{m=-l}^{l} \int_R d\vec{r} \sum_{g'} \mathscr{F}_{l,m}^{g'}(\vec{r}) \cdot \sum_g \delta\sigma^l(\vec{r}, g' \to g) \psi_{l,m}^g(\vec{r})$$

$$+ \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r} \, \psi_g(\vec{r}, \vec{\Omega}) \delta Q_g(\vec{r}, \vec{\Omega}) + \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r} \, \mathscr{F}_g(\vec{r}, \vec{\Omega}) \delta P_g(\vec{r}, \vec{\Omega}) \tag{13}$$

Equation (13) is the desired perturbation expression for a system with fixed sources. This equation gives the change in the functional $F$ for a given physical process due to changes in various neutron cross sections, changes in the fixed source, and changes in the physical process itself. This equation can also be used to give the change in $F$ due to perturbations in the individual material constituents of a shield layer or due to perturbations in individual neutron cross sections. Equation (13) is an exact relationship since no approximations are inherent in its derivation. However, since only low-order

perturbation theory is being considered, the perturbed flux $\mathscr{F}_g(\vec{r}, \vec{\Omega})$ may be replaced by its unperturbed value $\phi_g(\vec{r}, \vec{\Omega})$.

In shielding analysis, generally the biological dose rate at a detector position $\vec{r}_d$ is the functional of greatest interest. The interaction cross sections $P_g(\vec{r}, \vec{\Omega})$ are the flux-to-dose conversion factors which are independent of $\vec{r}$ and $\vec{\Omega}$. Thus, we can express $P_g(\vec{r}, \vec{\Omega})$ as

$$P_g(\vec{r}, \vec{\Omega}) = \frac{d_g}{4\pi} \tag{14}$$

where $d_g$ is the flux-to-dose conversion factor for group g. Insertion of equation (14) into equation (4b) gives

$$F = \frac{1}{4\pi} \sum_g d_g \Phi_g(\vec{r}_d) \tag{15}$$

Thus, the dose functional F is $1/4\pi$ times the dose rate at position $\vec{r}_d$.

The first two terms on the right side of equation (13), which depend on the density, can be put in terms of a material efficiency function $h^q(\vec{r})$ (ref. 8). That is, these terms can be defined as

$$4\pi\delta F_\sigma = \sum_q \int_R h^q(\vec{r}) \delta\rho^q(\vec{r})\, d\vec{r} \tag{16}$$

where q indicates a given material component and $\delta F_\sigma$ is the contribution of these terms to $\delta F$. The efficiency function $h^q(\vec{r})$ defines the change in the functional F caused by the introduction of a unit quantity of material q at position $\vec{r}$. The efficiency functions are derived in the appendix for the various terms which depend on the neutron cross sections. The efficiency functions are useful for determining the effect on F of the different material components of a region at any position within that region; also they are useful for determining the effect on F of the important neutron interactions which occur for a given material.

The calculational procedure used in applying the perturbation method to determine changes in neutron and gamma doses due to changes in shield layers is as follows:

(1) For an initial, layered shield configuration, solve equation (1) along with the boundary condition (eq. (2)) for the angular flux $\phi_g(\vec{r}, \vec{\Omega})$.

(2) Solve equation (5) along with the boundary condition (eq. (6)) for the angular dose importance function $\psi_g(\vec{r}, \vec{\Omega})$. This solution is for an inhomogeneous adjoint source at a detector location and for a set of flux-to-dose conversion factors.

(3) Compute the dose functional F by equations (3) and (10). The functionals F, obtained from these two equations, must be equal; differences are caused by the numerical approximations used in obtaining the angular fluxes and dose importances.

(4) Compute, by using equation (13), the change in the dose functional $\delta F$ caused by perturbations in the cross sections (due to density perturbations), perturbations in the fixed source, and perturbations in the dose response functions. The quantity $\delta F$ is computed separately for each shield layer for a nominal change in the layer density $\delta \rho$.

(5) The effect of each shield layer on F can be expressed as the fractional change in the dose functional per unit change in layer thickness $\delta F / F \delta t$. The coefficient $\delta F / F \delta t$ is determined by taking $\delta F$, computed for a nominal change in the density of a shield layer $\delta \rho$, and dividing by the product of the functional F and the change in the thickness of the shield layer $\delta t$. This change in the thickness of a shield layer $\delta t$ is related to a change in the density of a shield layer by $\delta t = \delta \rho t / \rho$ where $\rho$ is the density of the shield layer and t is its thickness; that is, by taking the product $\rho t$ as a constant.

## ILLUSTRATIVE PROBLEM

Some of the capabilities of the perturbation method are illustrated on the one-dimensional spherical system shown in figure 1. This system has a central cavity or void region with a radius of 30 centimeters followed by a 15-centimeter-thick layer of tungsten (W) and a 60-centimeter-thick layer of lithium hydride (LiH). A neutron source of $1.7 \times 10^{17}$ neutrons per second having a fission spectrum was uniformly distributed in the cavity. Doses and dose importance functions were evaluated for a detector located 0.25 centimeter from the outer boundary of the system. The composition of the system is listed in table I.

Neutron fluxes and importance values throughout the system were determined by using the $S_n$ method to solve both the forward and appropriate inhomogeneous adjoint equations. A 26-energy-group split was used to represent the neutron spectra. Elastic scattering was treated through the $P_3$ order. An $S_{16}$ Gauss-Legendre quadrature was utilized in these calculations.

The perturbation method was applied to secondary gamma sources - treating sources from neutron captures and from inelastic scatters individually. This necessitated generating each of these sources from neutron absorption and neutron inelastic scatter reaction rates in the tungsten layer (secondary gamma sources in the lithium hydride layer
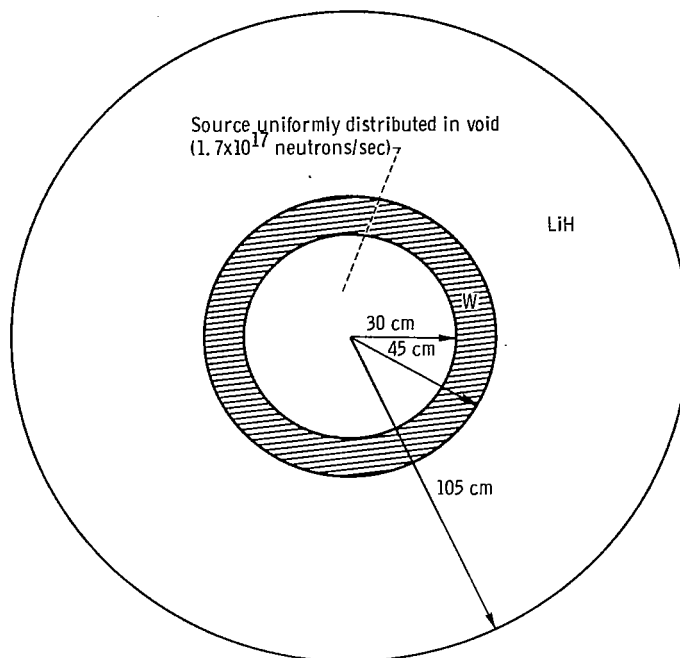
Figure 1. - One-dimensional spherical system used in illustrative problem.
(Detector position at 0. 25 cm from outer LiH boundary. )

TABLE I. - COMPOSITION OF

SPHERICAL SYSTEM

| Region | Element | Density, g cm$^3$ | Atom density, atom·b-cm |
|--------|---------|-------------------|--------------------------|
| 1 | (a) | - - - - - - - | - - - - - - - - |
| 2 | W | 19.27 | 0.0631 |
| | $W^{182}$ | 5.04 | 0.0167 |
| | $W^{183}$ | 2.77 | .0091 |
| | $W^{184}$ | 5.92 | .0194 |
| | $W^{186}$ | 5.54 | .0179 |
| 3 | LiH | 0.748 | 0.0568 |
| | $Li^6$ | 0.042 | 0.0042 |
| | $Li^7$ | .612 | .0526 |
| | H | .094 | .0568 |

$^a$Void.

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were neglected) and evaluating separately capture gamma and inelastic scatter gamma fluxes; the importance function for the gamma dose is independent of the gamma source component and is evaluated only once. $S_n$ transport calculations using a 15-energy-group split to represent the gamma spectra were made in a manner similar to those made for neutrons. In general, the perturbation method could more easily be applied by using a 41-energy-group coupled neutron-gamma $S_n$ transport calculation if the intent were to determine effects of shield layers on the combined neutron and gamma dose rates.

The effect of varying the density of each layer can be expressed as the fractional change in dose functional per unit change in layer thickness $\delta F/F\delta t$. These quantities are evaluated and compared with results obtained from successive direct calculations in which nominal changes in the thickness of each layer were made. The effects of various interactions in both shield layers on these dose derivatives are evaluated, as well as the influence of various material components of each layer.

Additional information is obtained from evaluating the perturbation equations for the neutron and gamma dose functions. This information is given in terms of a dose efficiency function which is the derivative of the dose functional with respect to weight and is evaluated as a function of position in each layer.

# RESULTS

## Effect of Tungsten and Lithium Hydride Layers on Neutron Dose

The neutron dose rate was calculated from equation (3) to be $2.90\times10^2$ rem per hour for the source of $1.7\times10^{17}$ neutrons per second. The neutron dose calculated from equation (10) was computed to be $3.11\times10^2$ rem per hour. The ratio of the dose calculated from equations (10) and (3) was equal to 1.07. This ratio should be unity, and departure from unity is a measure of the approximations inherent in the $S_n$ method for a given spatial mesh and angular quadrature. Thus, if the values of the dose functionals differ by a large enough amount to preclude obtaining the accuracy desired, then $S_n$ calculated angular fluxes and importances must be recalculated with a finer spatial mesh and angular quadrature.

For the illustrative problem considered, the importance function $\Psi_g(\vec{r})$ gives the dose at the detector due to a unit isotropic spherical shell source of neutrons located at position $\vec{r}$ in energy group g. Since the qualitative features of this neutron dose importance function $\Psi_g(\vec{r})$ are less well-known that those for the flux $\Phi_g(\vec{r})$, the neutron importance function obtained as a solution to equation (5) is shown in figure 2 for groups 1, 5, 10, and 15. Results for the other neutron energy groups show similar spatial
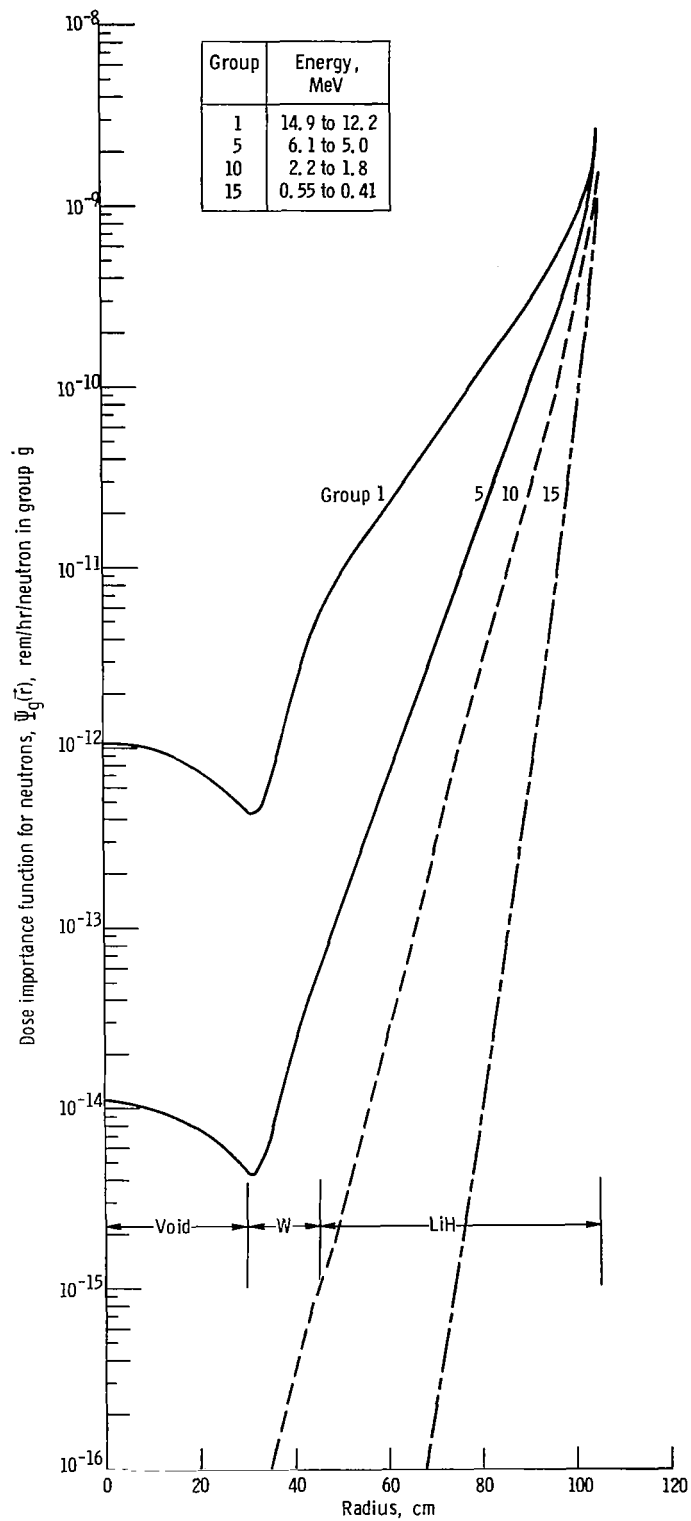
| Group | Energy, MeV |
|-------|-------------|
| 1 | 14.9 to 12.2 |
| 5 | 6.1 to 5.0 |
| 10 | 2.2 to 1.8 |
| 15 | 0.55 to 0.41 |

Figure 2. – Dose importance function for neutrons $\Psi_g(\bar{r})$, giving response of unit isotropic spherical shell sources. (Dose detector at 0.25 cm from outer boundary.)

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characteristics. Figure 2 indicates the strong effect of the LiH on the variation of the neutron dose importance function and the marked effect with energy group.

The effect of the tungsten layer on the neutron dose is presented in table II in terms of a coefficient $\delta F/F\delta t$ which gives the fractional change in the neutron dose per centimeter. The data in table II give the effect of the important reactions which a neutron can undergo with nuclei of tungsten. Inelastic neutron scattering accounts for 61 percent of the contribution to the effect of the tungsten layer, elastic neutron scattering contributes 20 percent, (n, 2n) reactions contribute 19 percent, and neutron absorptions have a negligible contribution.

TABLE II. - NEUTRON DOSE DERIVATIVES

$\delta F/F\delta t$ FOR TUNGSTEN LAYER,

COMPUTED BY PERTURBATION

THEORY

| Neutron reaction | Fractional change in neutron dose per centimeter, $\delta F/F\delta t$, $cm^{-1}$ |
|---|---|
| Elastic scattering | -0.047 |
| Inelastic scattering | -.146 |
| (n, 2n) Reaction | -.045 |
| Absorption | -.0001 |
| Total | -0.238 |

The effect of the lithium hydride layer on the neutron dose is presented in table III in terms of the coefficient $\delta F/F\delta t$. In addition, partial effects due to constituents hydrogen (H) and lithium (Li) are also presented. The data in table III indicate the dominant role of elastic neutron scattering for low-mass-number elements on the neutron dose functional. The data in the table also show that the effects of H and Li are nearly the same with respect to the neutron dose.

A comparison is given in table IV of the fractional change in the neutron dose functional per unit change in the tungsten layer thickness $\delta F/F\delta t$ between the perturbation theory result and the result calculated by successive direct transport calculations. The perturbation theory result is -0.238 $cm^{-1}$, while the result from direct flux calculations is -0.234 $cm^{-1}$. The two results are in close agreement with each other. For the LiH layer the perturbation theory result for the coefficient $\delta F/F\delta t$ is -0.138 $cm^{-1}$, while

TABLE III. - NEUTRON DOSE DERIVATIVES

$\delta F/F\delta t$  FOR LITHIUM HYDRIDE LAYER,

COMPUTED BY PERTURBATION THEORY

| Neutron reaction | Material | | |
|---|---|---|---|
| | H | Li | LiH |
| | Fractional change in neutron dose per centimeter, $\delta F/F\delta t$, $cm^{-1}$ | | |
| Elastic scattering | -0.070 | -0.040 | -0.110 |
| Inelastic scattering | ------ | -.027 | -.027 |
| Absorption | ------ | -.0005 | -.0005 |
| Total | -0.070 | -0.068 | -0.138 |

TABLE IV. - COMPARISON - FOR THE NEUTRON

PROBLEM - OF DERIVATIVE  $\delta F/F\delta t$

CALCULATED BY PERTURBATION

THEORY AND BY SUCCESSIVE

DIRECT TRANSPORT

CALCULATIONS

| Region | Fractional change in neutron dose per unit change in layer thickness, $\delta F/F\delta t$, $cm^{-1}$ | | Ratio of perturbation result to direct result |
|---|---|---|---|
| | Perturbation calculation | Direct calculation | |
| W | -0.238 | -0.234 | 1.02 |
| LiH | -.138 | -.140 | .99 |

the result obtained from direct flux calculations is -0.140 $cm^{-1}$.  Again the two results are in close agreement with each other.

In computing the perturbation theory results, material efficiency functions  $h(\vec{r})$  were generated as intermediate results for each material component and for each neutron reaction as a function of position within a layer.  This additional information can be used in other aspects of shield analysis since  $h(\vec{r})$  is a derivative giving the change in the dose functional  F  per unit mass of material introduced at position  $\vec{r}$.  For this illustrative problem the total  $h(\vec{r})$  of each material component is shown in figure 3(a) for
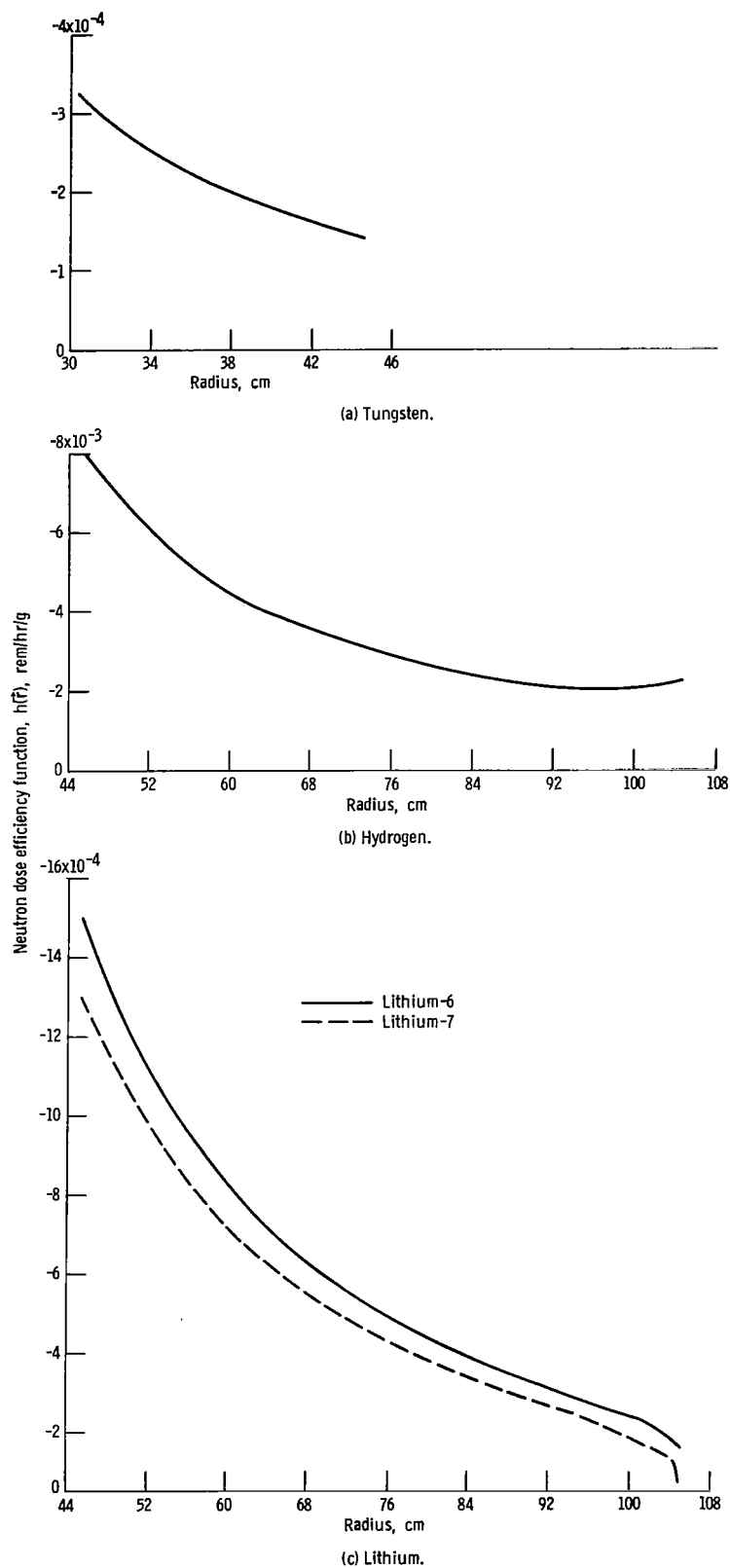
Figure 3. – Total neutron dose efficiency functions for tungsten, hydrogen, and lithium.

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the W of the W layer and in figures 3(b) and (c) for the H, $Li^6$, and $Li^7$ components of the LiH layer.

## Effect of Tungsten and Lithium Hydride Layers on Secondary Gamma Dose

The gamma-ray dose rate was calculated from equation (3) to be $2.59 \times 10^4$ rads per hour for a gamma-ray source due to neutron absorptions in W of $3.98 \times 10^{17}$ photons per second. By using equation (10) the gamma dose was also calculated to be $2.59 \times 10^4$ rads per hour. The gamma-ray dose was calculated from equation (3) to be $7.10 \times 10^3$ rads per hour for a gamma-ray source due to neutron inelastic scattering in W of $8.17 \times 10^{17}$ photons per second. From equation (10) the photon dose for this case was calculated to be $7.19 \times 10^3$ rads per hour.

The gamma-ray dose importance function $\Psi_g(\vec{r})$ is shown in figure 4 for energy groups 1, 5, and 10. Results for the other photon energy groups show similar spatial characteristics. Figure 4 indicates the strong effect of the W on the variation of the gamma-ray importance function.

The secondary source distributions due to $W(n, \gamma)$ and $W(n, n'\gamma)$ reactions are shown in figure 5(a). The perturbation formula (eq. (13)) for the secondary gamma source includes a term which is based on the difference between the perturbed and unperturbed neutron fluxes. This perturbed secondary source term is estimated in the following manner: The neutron transport problem is calculated as a two-outer-iteration problem. The first iteration is performed for a small perturbation in the density of the W layer. This yields a set of perturbed neutron fluxes which are stored. The density of W is next restored to its unperturbed value, and the calculation continues as a second outer iteration for the unperturbed neutron fluxes. The difference between the perturbed and unperturbed values of the neutron fluxes are then used to calculate the perturbations in the secondary sources. Figure 5(b) presents the perturbations in the secondary source distributions for the $W(n, \gamma)$ and $W(n, n'\gamma)$ reactions for a 1-percent increase in the density of the W layer. In a coupled neutron-gamma problem the secondary gamma sources never explicitly appear in the equations and the preceding source perturbation calculation is not necessary.

The effect of the tungsten layer on the gamma doses is presented in table V in terms of the coefficient $\delta F/F\delta t$. The data in table V give the effect of each reaction which a gamma ray can undergo with a nuclei of W. In addition, the effect on the gamma dose of perturbations in the secondary gamma-ray source is also given. The data show that these perturbations in the secondary gamma source are a major contribution to the gamma dose functional. The effect of the LiH layer on the gamma doses is presented
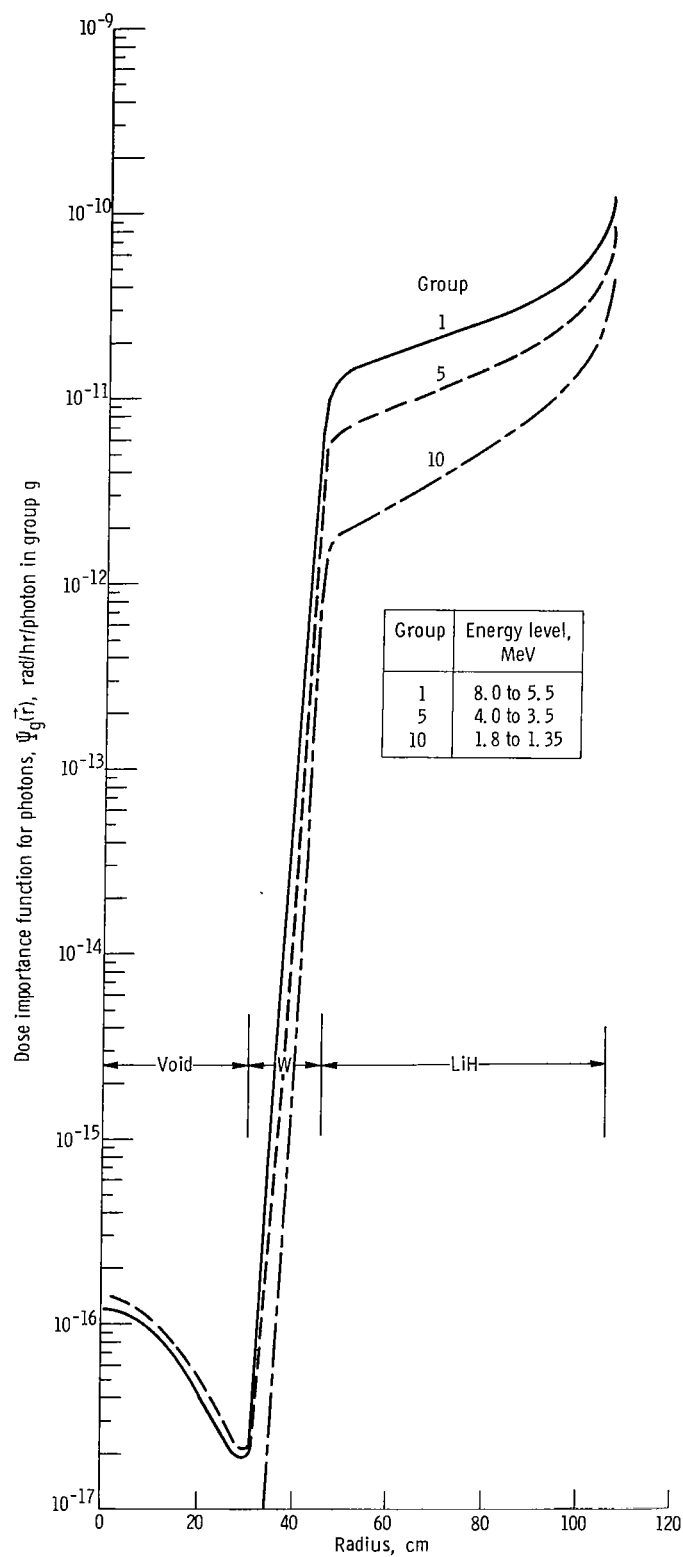
Figure 4. – Dose importance function for photons $\Psi_g(\vec{r})$, giving response of unit isotropic spherical shell sources. (Dose detector at 0.25 cm from outer boundary.)
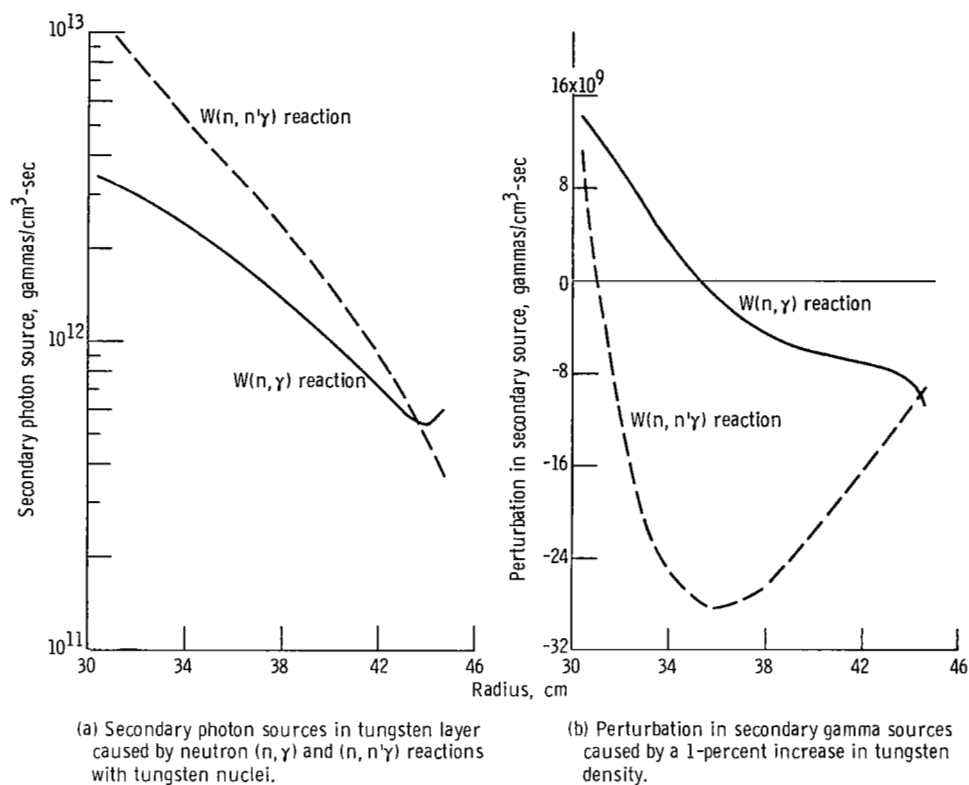
| Group | Energy level, MeV |
|-------|-------------------|
| 1     | 8.0 to 5.5        |
| 5     | 4.0 to 3.5        |
| 10    | 1.8 to 1.35       |

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(a) Secondary photon sources in tungsten layer caused by neutron (n, γ) and (n, n'γ) reactions with tungsten nuclei.

(b) Perturbation in secondary gamma sources caused by a 1-percent increase in tungsten density.

Figure 5. – Secondary source distributions.

TABLE V. - SECONDARY GAMMA DOSE DERIVATIVES

$\delta F/F\delta t$ FOR TUNGSTEN LAYER, COMPUTED BY

PERTURBATION THEORY

| | Secondary photon source | |
|---|---|---|
| | $W(n, \gamma)$ reaction | $W(n, n'\gamma)$ reaction |
| | Fractional change in photon dose per centimeter, $\delta F/F\delta t$, $cm^{-1}$ | |
| Photon reaction: | | |
| Scattering | -0.041 | -0.068 |
| Absorption | -.029 | -.022 |
| Secondary source perturbations | -.040 | -.082 |
| Total | -0.110 | -0.172 |

TABLE VI. - SECONDARY GAMMA DOSE DERIVATIVES δF/Fδt FOR

LITHIUM HYDRIDE LAYER, COMPUTED BY

PERTURBATION THEORY

| | Secondary photon source | | | | | |
|---|---|---|---|---|---|---|
| | W(n, $\gamma$) reaction | | | W(n, n'$\gamma$) reaction | | |
| | Material | | | | | |
| | H | Li | LiH | H | Li | LiH |
| | Fractional change in photon dose per unit change in layer thickness, δF/Fδt, cm$^{-1}$ | | | | | |
| Photon reaction: Scattering Absorption | -0.0065 (a) | -0.0195 (a) | -0.026 (a) | -0.010 (a) | -0.029 (a) | -0.039 (a) |
| Total | -0.0065 | -0.0195 | -0.026 | -0.010 | -0.029 | -0.039 |

[a]Negligible.


TABLE VII. - COMPARISON - FOR GAMMA

PROBLEM - OF DERIVATIVE δF/Fδt

CALCULATED BY PERTURBATION

THEORY AND BY SUCCESSIVE

DIRECT TRANSPORT

CALCULATIONS

| Region | Fractional change in photon dose per unit change in layer thickness, δF/Fδt, cm$^{-1}$ | | Ratio of perturbation result to direct result |
|---|---|---|---|
| | Perturbation calculation | Direct calculation | |
| Secondary photon source: W(n, $\gamma$) reaction | | | |
| W | -0.110 | -0.107 | 1.03 |
| LiH | -.026 | -.026 | 1.00 |
| Secondary photon source: W(n, n'$\gamma$) reaction | | | |
| W | -0.172 | -0.168 | 1.02 |
| LiH | -.039 | -.039 | 1.00 |

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in table VI in terms of the coefficient $\delta F/F \delta t$ for the two secondary gamma-ray sources.

The coefficient $\delta F/F \delta t$ as computed by perturbation theory and successive direct flux calculations is compared in table VII for the W and LiH layers. The table shows that the coefficient $\delta F/F \delta t$ computed by perturbation theory is in agreement with the result obtained from successive direct flux calculations for all cases.

The total material efficiency functions $h(\vec{r})$ with respect to the gamma-ray dose are shown in figures 6(a) and (b). These functions were obtained by using the perturbation equations for each material component of the LiH layer and for the W of the W layer.
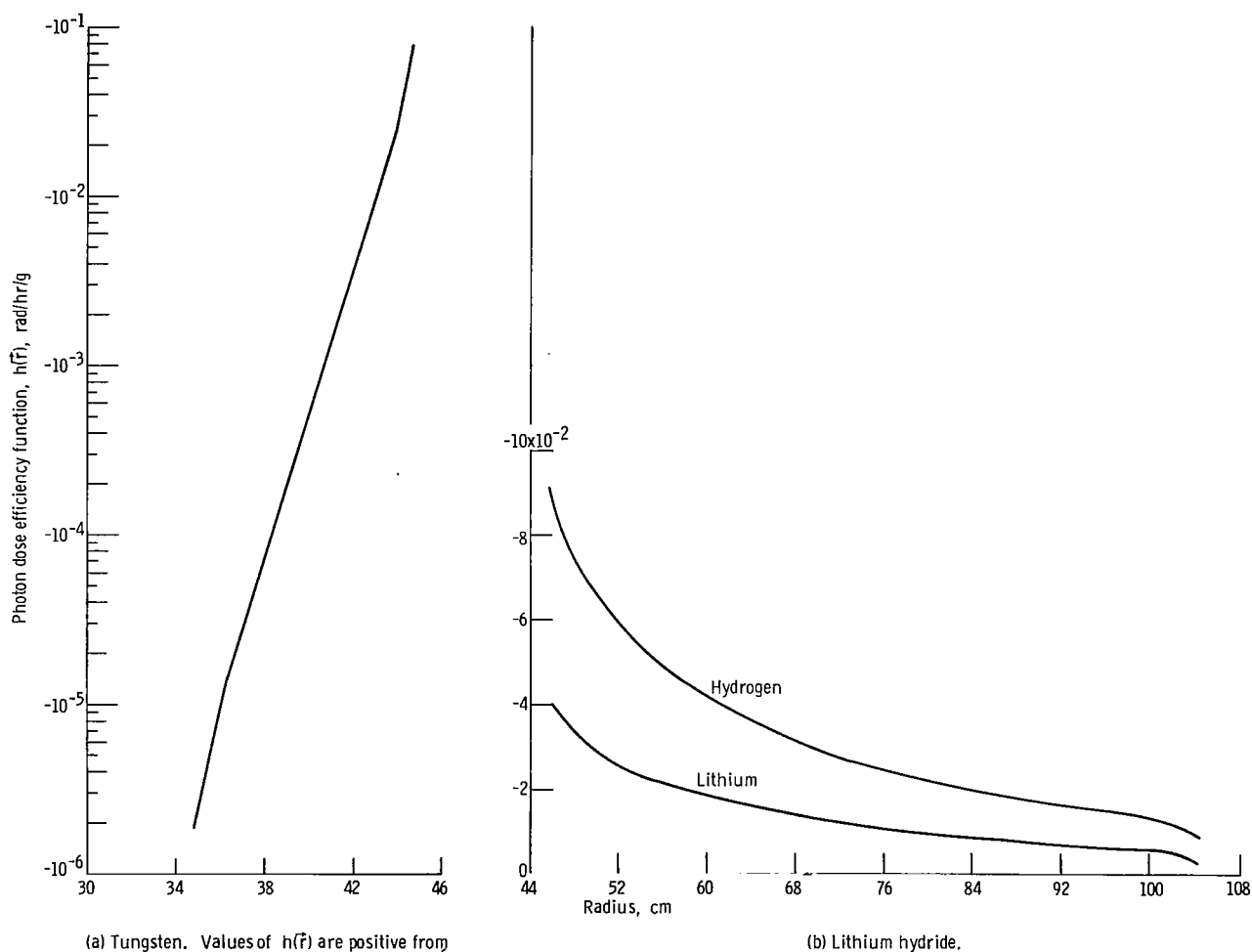


(a) Tungsten. Values of $h(\vec{r})$ are positive from 30- to 34-centimeter radius and of order $10^{-6}$.

(b) Lithium hydride.

Figure 6. – Total photon dose efficiency function for tungsten and for lithium hydrode. Secondary gamma source: $W(n, \gamma)$ reactions.

# CONCLUSIONS

The result for the coefficient $\delta F/F\delta t$ giving the fractional change in the dose per unit change in shield layer thickness that were obtained by using perturbation theory formulas for fixed sources were in excellent agreement with those obtained by using successive direct transport calculations. The perturbation method also gives a considerable amount of information concerning each reaction which a neutron or photon can undergo with the nuclei of various materials and thus adds to the qualitative understanding of changes in shield design. This same information is not easily or readily obtainable from successive direct transport calculations. Although the features of this perturbation method were exhibited with a simple one-dimensional spherical problem, the extension of the perturbation method to two-dimensional geometry and to coupled neutron - gamma-ray problems poses no additional difficulty.

Lewis Research Center,
   National Aeronautics and Space Administration,
      Cleveland, Ohio, September 1, 1972,
         503-05.

# APPENDIX - PERTURBATION THEORY FOR SYSTEMS WITH FIXED SOURCES

## Neutron Transport Equation

The application of perturbation theory in the computation of reactivity effects is well known and, in fact, was used from the very beginning of the atomic energy program. Less well known is the application of perturbation theory to the computation of nonreactivity effects such as, for example, the breeding ratio of a reactor system, the sensitivity of the biological dose rate to variations in shield composition, and the sensitivity of other reactor processes to variations in the system. The theory underlying the application of perturbation methods to such nonreactivity problems appear mainly in the Russian literature (refs. 7 and 8). Lewins reviews, in reference 6, this and other developments in perturbation theory. This appendix gives the details of the mathematical analysis underlying the use of perturbation theory for systems with fixed sources. The symbols used are mainly conventional; those that are not are defined.

To provide a theoretical basis for understanding perturbation theory for systems with fixed sources, consider the time-independent multigroup form of the neutron transport equation. This equation is given by

$$\vec{\Omega} \cdot \vec{\nabla} \phi_g(\vec{r}, \vec{\Omega}) + \sigma_g(\vec{r}) \phi_g(\vec{r}, \vec{\Omega}) = Q_g(\vec{r}, \vec{\Omega}) + \frac{1}{4\pi} \sum_{g'} \sigma(\vec{r}, g' \to g) \Phi_{g'}(\vec{r})$$

$$+ \sum_{l=1}^{\infty} \frac{2l+1}{4\pi} \cdot \sum_{g'} \Sigma_{es}^l(\vec{r}, g' \to g) \cdot \sum_{m=-l}^{l} \phi_{l,m}^{g'}(\vec{r}) P_{l,m}(\vec{\Omega}) \qquad g = 1, 2, \ldots, G \qquad (A1)$$

where $\phi_g(\vec{r}, \vec{\Omega})$ is the angular flux for group g, $\sigma_g$ is the macroscopic total cross section for group g, $Q_g(\vec{r}, \vec{\Omega})$ is the angular fixed source for group g, $\sigma^l(g' \to g)$ is the $l^{th}$-order macroscopic cross section for scattering from group g' to group g, $\phi_{l,m}^g(\vec{r})$ is the $(l, m)^{th}$ expansion coefficient of the angular flux of group g in a spherical harmonic series, and $P_{l,m}(\vec{\Omega})$ is the $(l, m)^{th}$ spherical harmonic as a function of the unit direction vector $\vec{\Omega}$.

For convenience in performing subsequent manipulations, the equation is written for one material component. In reality, all the terms involving cross sections in equation (A1) are summations for all the material components present at position $\vec{r}$. Although equation (A1) will be studied from the point of view of neutron transport, it is apparent that the analysis will also pertain to photon transport or coupled neutron and gamma-ray transport when a proper identification of terms is made. This is essential,

for example, in determining the biological dose rate external to a reactor shield which is composed of both a neutron and photon component.

In deriving equation (A1) the angular flux which occurs in the elastic scattering integral on the right side of the equation has been expanded in a series of spherical harmonics and is given by

$$\phi_g(\vec{r}, \vec{\Omega}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{2l + 1}{4\pi} \phi_{l,m}^g(\vec{r}) P_{l,m}(\vec{\Omega}) \tag{A2}$$

The spherical harmonics are defined here as

$$P_{l,m}(\vec{\Omega}) = \left[ \frac{(2 - \delta_{mo})(l - m)!}{(l + m)!} \right]^{1/2} \cdot P_l^m(\mu) \cos(m\varphi) \qquad l \geq 0, \ 0 \leq m \leq l \tag{A3a}$$
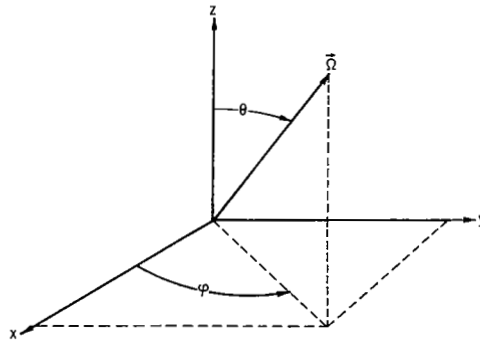
and

$$P_{l,-m}(\vec{\Omega}) = \left[ \frac{2(l - m)!}{(l + m)!} \right]^{1/2} \cdot P_l^m(\mu) \sin(m\varphi) \qquad l > 0, \ 0 < m \leq l \tag{A3b}$$

where $P_l^m(\mu)$ are the associated Legendre polynomials of argument $\mu$ and where $\delta_{mo}$ is the Kronecker delta which has the property that

$$\delta_{kk'} = \begin{cases} 1 & k = k' \\ 0 & k \neq k' \end{cases} \tag{A4}$$

For the local Cartesian coordinate system at position $\vec{r}$ shown in the following sketch (where $\theta$ is the polar angle and $\varphi$ is the azimuthal angle), $\mu = \cos \theta$.

Thus, from the sketch, the unit vector $\vec{\Omega}$ is given by

$$\vec{\Omega} = \vec{\Omega}(\mu, \varphi) \tag{A5}$$

and the element of solid angle $d\Omega$ given by

$$d\Omega = d\mu \, d\varphi \tag{A6}$$

For geometries with symmetry in the azimuthal angle $\varphi$, all the terms in $\sin(m\varphi)$ are identically zero in the expansion of the angular flux. Thus, the complexity of equation (A2) is reduced for simple geometries. For example, only the terms in $P_{l,0}(\vec{\Omega})$ - the Legendre polynomials - are needed for one-dimensional slab or spherical geometry.

The spherical harmonics defined here have two important properties. One of these is the orthogonality property given by

$$\int_{\vec{\Omega}} P_{l,m}(\vec{\Omega}) P_{l',m'}(\vec{\Omega}) \, d\Omega = \frac{4\pi}{2l+1} \, \delta_{ll'} \delta_{mm'} \tag{A7}$$

The other property is the addition theorem, which is given by the equation

$$P_l(\vec{\Omega} \cdot \vec{\Omega}') = \sum_{m=-l}^{l} P_{l,m}(\vec{\Omega}) P_{l,m}(\vec{\Omega}') \tag{A8}$$

By the orthogonality property of these spherical harmonics, the $\phi^g_{l,m}(\vec{r})$ of equation (A2) can be determined. These are given by

$$\phi^g_{l,m}(\vec{r}) = \int_{\vec{\Omega}} \phi_g(\vec{r}, \vec{\Omega}) P_{l,m}(\vec{\Omega}) \, d\Omega \tag{A9}$$

The quantity $\phi^g_{0,0}(\vec{r})$ is the scalar neutron flux for group g and will be represented more simply as $\Phi_g(\vec{r})$. The net neutron current vector $\vec{J}_g(\vec{r})$ is given by the equation

$$\vec{J}_g(\vec{r}) = \int_{\vec{\Omega}} \phi_g(\vec{r}, \vec{\Omega}) \vec{\Omega} \, d\Omega$$

$$= \hat{i}\phi^g_{1,1}(\vec{r}) + \hat{j}\phi^g_{1,-1}(\vec{r}) + \hat{k}\phi^g_{1,0}(\vec{r}) \tag{A10}$$

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where $\hat{i}$, $\hat{j}$, and $\hat{k}$ are unit vectors along the x-, y-, and z-coordinate axes, respectively.

The unit vector $\vec{\Omega}$ is given in terms of the spherical harmonics by

$$\vec{\Omega} = \hat{i} \, P_{1,\,1}(\vec{\Omega}) + \hat{j} \, P_{1,\,-1}(\vec{\Omega}) + \hat{k} \, P_{1,\,0}(\vec{\Omega}) \tag{A11}$$

Equations (A10) and (A11) can next be combined to give the dot product of $\vec{\Omega}$ and $\vec{J}_g(\vec{r})$. This is

$$\vec{\Omega} \cdot \vec{J}_g(\vec{r}) = \sum_{m=-1}^{1} \phi_{1,\,m}^{g}(\vec{r}) P_{1,\,m}(\vec{\Omega}) \tag{A12}$$

To complete the description of equation (A1), we must recall that a number of quantities must satisfy certain normalization requirements. These are

$$\Sigma_{es,\,g} = \sum_{g'} \Sigma_{es}^{o}(g \rightarrow g') \tag{A13a}$$

$$\Sigma_{in,\,g} = \sum_{g'} \Sigma_{in}(g \rightarrow g') \tag{A13b}$$

$$\Sigma_{n2n,\,g} = \frac{1}{2} \sum_{g'} \Sigma_{n2n}(g \rightarrow g') \tag{A13c}$$

$$\langle \mu_L \rangle_g \cdot \Sigma_{es,\,g} = \sum_{g'} \Sigma_{es}^{1}(g \rightarrow g') \tag{A13d}$$

$$\langle P_l(\mu_L) \rangle_g \cdot \Sigma_{es,\,g} = \sum_{g'} \Sigma_{es}^{l}(g \rightarrow g') \tag{A13e}$$

Note also that, when neutron leakage is treated by means of a buckling term, the quantity $\sigma_g(\vec{r})$ must be suitably modified. The quantities $\Sigma_{es,\,g}$, $\Sigma_{in,\,g}$, and $\Sigma_{n2n,\,g}$ are the macroscopic elastic, inelastic, and (n, 2n) cross sections for group g, respectively. The quantities $\langle \mu_L \rangle_g$ and $\langle P_l(\mu_L) \rangle_g$ represent the average cosine and the average $l$ [th] order Legendre polynomial of elastic scattering for group g, respectively.

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# Functional for a Physical Process

A physical process which can occur in a system described by equation (A1) and which depends linearly on the angular flux can be written as a functional $F$ which is given in multigroup form by

$$F = \sum_g F_g = \sum_g \int_{\bar{\Omega}} \int_R \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) \, d\vec{r} d\Omega \tag{A14}$$

where $F_g$ is given by

$$F_g = \int_{\bar{\Omega}} \int_R \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) \, d\vec{r} d\Omega \tag{A15}$$

The functional $F$ gives contributions caused by the physical process for the neutrons in the system. The quantity $P_g(\vec{r}, \vec{\Omega})$ has the role of an interaction cross section for the physical process occurring in group g at position $\vec{r}$ for neutrons moving in the direction $\vec{\Omega}$. The integrations in equations (A14) and (A15) are over all directions $\bar{\Omega}$ and for the entire system designated as R.

If a functional at some specific point, $\vec{r}_d$, is required, equation (A14) can be written as

$$F(\vec{r}_d) = \sum_g \int_{\bar{\Omega}} \int_R \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) \delta(\vec{r} - \vec{r}_d) \, d\vec{r} d\Omega \tag{A16a}$$

$$F(\vec{r}_d) = \sum_g \int_{\bar{\Omega}} \phi_g(\vec{r}_d, \vec{\Omega}) P_g(\vec{r}_d, \vec{\Omega}) \, d\Omega \tag{A16b}$$

where $\delta(\vec{r} - \vec{r}_d)$ is the Dirac delta function. The general expression, equation (A14), will be used in subsequent derivations. Equation (A16a) will be invoked when results such as radiation dose at a given position are required.

In shielding analysis, as an example, generally the biological dose rate at a detector position $\vec{r}_d$ is the functional of greatest interest. The interaction cross sections $P_g(\vec{r}, \vec{\Omega})$ are the flux-to-dose conversion factors which are independent of $\vec{r}$ and $\vec{\Omega}$. Thus, $P_g(\vec{r}, \vec{\Omega})$ can be expressed as

$$P_g(\vec{r}, \vec{\Omega}) = \frac{d_g}{4\pi} \qquad (A17)$$

where $d_g$ is the flux-to-dose conversion factor for group g. Insertion of equation (A17) into equation (A16b) gives

$$F = \frac{1}{4\pi} \sum_g d_g \Phi_g(\vec{r}_d) \qquad (A18)$$

Thus, for this shielding application, the functional F is $1/4\pi$ times the dose rate at position $\vec{r}_d$.

## Importance Equation for a Given Physical Process

Following Usachev (ref. 7), an equation can be derived for the importance of neutrons for a given physical process. The importance of an initial distribution of neutrons is equal to the sum of the importance of all the scattered neutrons and of the number of processes which occur. Since the importance of each process is, by definition, unity, the preceding statement results in a law of conservation of importance. Therefore, let $\psi_g(\vec{r}, \vec{\Omega})$ be the importance of a neutron introduced in group g at position $\vec{r}$ and moving in the direction $\vec{\Omega}$. If $\vec{r}'$ corresponds to the position of a neutron in group g after it travels a distance ds in the direction $\vec{\Omega}$ at position $\vec{r}$, then the following expression gives the importance due to M neutrons:

$M\psi_g(\vec{r}, \vec{\Omega}) = M\psi_g(\vec{r}', \vec{\Omega}) \cdot$ (Probability that a neutron does not have a collision in ds)

+ (Importance due to scattered neutrons produced by original neutrons in distance ds)

+ (Importance of physical process in distance ds) $\qquad$ (A19)

The terms on the right side of equation (A19) which are expressed in words can be easily given in terms of multigroup cross sections, that is,

$$M\psi_g(\vec{r}, \vec{\Omega}) = M \cdot \left[1 - \sigma_g(\vec{r})ds\right]\psi_g(\vec{r}', \vec{\Omega}) + \frac{Mds}{4\pi} \cdot \sum_{g'} \sigma(\vec{r}, g{\to}g')\Psi_{g'}(\vec{r})$$

$$+ Mds \cdot \sum_{l=1}^{\infty} \frac{2l+1}{4\pi} \cdot \sum_{g'} \Sigma_{es}^{l}(\vec{r}, g{\to}g') \cdot \sum_{m=-l}^{l} \psi_{l,m}^{g'}(\vec{r})P_{l,m}(\vec{\Omega})$$

$$+ Mds \cdot P_g(\vec{r}, \vec{\Omega}) \cdot \text{(Unit importance)} \tag{A20}$$

Next expand $\psi_g(\vec{r}', \vec{\Omega})$ in a Taylor's series about $\vec{r}$:

$$\psi_g(\vec{r}', \vec{\Omega}) \doteq \psi_g(\vec{r}, \vec{\Omega}) + \frac{\partial\psi_g(\vec{r}, \vec{\Omega})}{\partial s} ds + O(ds)^2 \tag{A21}$$

Also make the following replacement:

$$\frac{\partial\psi_g(\vec{r}, \vec{\Omega})}{\partial s} = \vec{\Omega} \cdot \vec{\nabla}\psi_g(\vec{r}, \vec{\Omega}) \tag{A22}$$

Substitute equation (A21) into equation (A20), divide through by $Mds$, and let $ds \to 0$. The result will be an integrodifferential equation for the importance of neutrons to the given physical process. This equation is given by

$$-\vec{\Omega} \cdot \vec{\nabla}\psi_g(\vec{r}, \vec{\Omega}) + \sigma_g(\vec{r})\psi_g(\vec{r}, \vec{\Omega}) = \frac{1}{4\pi} \sum_{g'} \sigma(\vec{r}, g{\to}g')\Psi_{g'}(\vec{r})$$

$$+ \sum_{l=1}^{\infty} \frac{2l+1}{4\pi} \cdot \sum_{g'} \Sigma_{es}^{l}(\vec{r}, g{\to}g') \cdot \sum_{m=-l}^{l} \psi_{l,m}^{g'}(\vec{r})P_{l,m}(\vec{\Omega})$$

$$+ P_g(\vec{r}, \vec{\Omega}) \qquad g = 1, 2, \ldots, G \tag{A23}$$

Although equation (A23) is, in the strictest sense, not adjoint to equation (A1), it is adjoint-like in that it gives the importance of neutrons for the physical process. Note that different interaction processes described by the function $P_g(\vec{r}, \vec{\Omega})$ result in different importance functions $\psi_g(\vec{r}, \vec{\Omega})$.

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The boundary condition for the importance $\psi_g(\vec{r}, \vec{\Omega})$ follows from the fact that, if a neutron escapes from a system, it cannot contribute to the physical process. Therefore, its importance must be zero and the boundary condition becomes

$$\psi_g(\vec{r}_s, \vec{\Omega}^+) = 0 \qquad g = 1, 2, \ldots, G \tag{A24}$$

where $\vec{r}_s$ indicates the outer boundary of the system and $\vec{\Omega}^+$ designates an outward direction.

In deriving equation (A23) and in analogy with equation (A1), the importance function which occurs in the elastic scattering integral on the right side of the equation has been expanded in a series of spherical harmonics and is given by

$$\psi_g(\vec{r}, \vec{\Omega}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{2l+1}{4\pi} \psi_{l,m}^g(\vec{r}) P_{l,m}(\vec{\Omega}) \tag{A25}$$

By the orthogonality of the spherical harmonics used here, the $\psi_{l,m}^g(\vec{r})$ of equation (A25) can be determined. They are given by

$$\psi_{l,m}^g(\vec{r}) = \int_{\vec{\Omega}} \psi_g(\vec{r}, \vec{\Omega}) P_{l,m}(\vec{\Omega}) \, d\Omega \tag{A26}$$

The quantity $\psi_{0,0}^g(\vec{r})$ is the scalar importance for group g and will be represented more simply as $\Psi_g(\vec{r})$. A vector $\vec{J}_g^+(r)$, which is the net importance current vector, is defined by the equation

$$\vec{J}_g^+(r) = \int_{\vec{\Omega}} \psi_g(\vec{r}, \vec{\Omega}) \vec{\Omega} \, d\Omega = \hat{i}\psi_{1,1}^g(\vec{r}) + \hat{j}\psi_{1,-1}^g(\vec{r}) + \hat{k}\psi_{1,0}^g(\vec{r}) \tag{A27}$$

Equations (A11) and (A27) can be combined to yield the dot product of $\vec{\Omega}$ and $\vec{J}_g^+(r)$, that is,

$$\vec{\Omega} \cdot \vec{J}_g^+(r) = \sum_{m=-1}^{1} \psi_{1,m}^g(\vec{r}) P_{1,m}(\vec{\Omega}) \tag{A28}$$

# Perturbation Equation for a Given Physical Process

Consider a system which is perturbed in a manner such that all the cross sections are varied. The solution of equation (A1) with the perturbed cross sections yields a perturbed value for the angular flux. The neutron transport equation for this case is given by

$$\vec{\Omega} \cdot \vec{\nabla} \mathscr{F}_g(\vec{r}, \vec{\Omega}) + \left[ \sigma_g(\vec{r}) + \delta\sigma(\vec{r}) \right] \cdot \mathscr{F}_g(\vec{r}, \vec{\Omega}) = \frac{1}{4\pi} \cdot \sum_{g'} \left[ \sigma(\vec{r}, g' \to g) + \delta\sigma(\vec{r}, g' \to g) \right] \cdot \mathscr{F}_{g'}(\vec{r})$$

$$+ \sum_{l=1}^{\infty} \frac{2l+1}{4\pi} \cdot \sum_{g'} \left[ \Sigma_{es}^l(\vec{r}, g' \to g) + \delta\Sigma_{es}^l(\vec{r}, g' \to g) \right] \cdot \sum_{m=-1}^{l} \mathscr{F}_{l,m}^{g'}(\vec{r}) P_{l,m}(\vec{\Omega})$$

$$+ Q_g(\vec{r}, \vec{\Omega}) + \delta Q_g(\vec{r}, \vec{\Omega}) \qquad g = 1, 2, \ldots, G \tag{A29}$$

In the preceding equation $\mathscr{F}_g(\vec{r}, \vec{\Omega})$ represents the perturbed value of the angular flux for group g. Perturbations in the cross sections are indicated by replacing a cross section $\sigma$ by $\sigma + \delta\sigma$ where $\delta\sigma$ is the perturbation. The source term $Q_g(\vec{r}, \vec{\Omega})$ is assumed to undergo a perturbation in the amount of $\delta Q_g(\vec{r}, \vec{\Omega})$.

Multiply equation (A29) by $\psi_g(\vec{r}, \vec{\Omega})$ and then integrate the resulting equation over all $d\vec{r}d\Omega$ as well as summing the results over all groups g. Next multiply equation (A23) by $\mathscr{F}_g(\vec{r}, \vec{\Omega})$ and then integrate the resulting equation over all $d\vec{r}d\Omega$ as well as summing the results over all groups g. Finally, subtract the second equation from the first; and the result, after considerable algebraic manipulation, will be

$$\sum_g \int_{\Omega} d\Omega \int_S \mathscr{F}_g(\vec{r}_s, \vec{\Omega}) \psi_g(\vec{r}_s, \vec{\Omega}) \vec{\Omega} \cdot \vec{n} \, dS + \sum_g \int_{\Omega} d\Omega \int_R d\vec{r} \, \delta\sigma_g(\vec{r}) \psi_g(\vec{r}, \vec{\Omega}) \mathscr{F}_g(\vec{r}, \vec{\Omega})$$

$$- \frac{1}{4\pi} \int_R d\vec{r} \sum_{g'} \mathscr{F}_{g'}(\vec{r}) \cdot \sum_g \delta\sigma(\vec{r}, g' \to g) \psi_g(\vec{r})$$

$$- \sum_{l=1}^{\infty} \frac{2l+1}{4\pi} \cdot \sum_{m=-l}^{l} \int_R d\vec{r} \sum_{g'} \mathscr{F}_{l,m}^{g'}(\vec{r}) \cdot \sum_g \delta\Sigma_{es}^l(\vec{r}, g' \to g) \psi_{l,m}^g(\vec{r})$$

$$- \sum_g \int_{\Omega} d\Omega \int_R d\vec{r} \, \psi_g(\vec{r}, \vec{\Omega}) Q_g(\vec{r}, \vec{\Omega}) - \sum_g \int_{\Omega} d\Omega \int_R d\vec{r} \, \psi_g(\vec{r}, \vec{\Omega}) \delta Q_g(\vec{r}, \vec{\Omega})$$

$$+ \sum_g \int_{\Omega} d\Omega \int_R d\vec{r} \, \mathscr{F}_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) = 0 \tag{A30}$$

In the first term of the preceding equation, dS is an element on the outer surface S of the system.

If all the perturbations in equation (A30) are zero, then the equation reduces to

$$\sum_g \int_{\vec{\Omega}} d\Omega \int_S \phi_g(\vec{r}_s, \vec{\Omega}) \psi_g(\vec{r}_s, \vec{\Omega}) \vec{\Omega} \cdot \vec{n}\, ds - \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \psi_g(\vec{r}, \vec{\Omega}) Q_g(\vec{r}, \vec{\Omega})$$

$$+ \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) = 0 \qquad (A31)$$

where $\mathscr{F}_g(\vec{r}, \vec{\Omega})$ has been replaced by its unperturbed value $\phi_g(\vec{r}, \vec{\Omega})$. Equation (A33) is well known and is the multigroup form of a similar equation as obtained by Hansen and Sandmeier (ref. 9).

The boundary condition for the angular flux at the convex boundary of the system will be taken as

$$\phi_g(\vec{r}_s, \vec{\Omega}^-) = 0 \qquad g = 1, 2, \ldots, G \qquad (A32)$$

This boundary condition is the usual condition implying that no neutrons enter the system from the vacuum. Here $\vec{\Omega}^-$ designates an inward direction. Using boundary conditions (A24) and (A32) reduces equation (A31) to

$$F = \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega})$$

$$= \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\, \psi_g(\vec{r}, \vec{\Omega}) Q_g(\vec{r}, \vec{\Omega}) \qquad (A33)$$

Equation (A33) shows that the functional F for a given physical process may be computed in two different ways. The equation may also be used to give another useful description for the importance function $\psi_g(\vec{r}, \vec{\Omega})$. Let the source $Q_g(\vec{r}, \vec{\Omega})$ be given by

$$Q_g(\vec{r}, \vec{\Omega}) = \delta(\vec{r} - \vec{r}_0)\delta(\vec{\Omega} - \vec{\Omega}_0)\delta_{gg'} \qquad (A34)$$

The source given by this equation describes a source of neutrons in group g' at position $\vec{r}_o$ and moving the direction $\vec{\Omega}_o$. Next substitute equation (A34) for $Q_g(\vec{r}, \vec{\Omega})$ in equation (A33). This will give

$$\psi_{g'}(\vec{r}_o, \vec{\Omega}_o) = \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r} \, \phi_g(\vec{r}, \vec{\Omega}) P_g(\vec{r}, \vec{\Omega}) \qquad (= F) \qquad (A35)$$

Equation (A35) leads to the conclusion that the importance function $\psi_g(\vec{r}, \vec{\Omega})$ is the functional for a physical process for a unit source of neutrons placed in group g at position $\vec{r}$ and traveling in direction $\vec{\Omega}$. In other words, the importance function $\psi_g(\vec{r}, \vec{\Omega})$ is a Green's function. Further, a solution of equation (A23) provides the functional for a physical process for every possible unit source. Equation (A35) gives the units of the importance function $\Psi_g(\vec{r})$ as that of the functional F per source particle.

From equation (A33) we can deduce the following additional conclusions concerning the functional F: If the value of the functional is needed for a number of different source distributions $Q_g(\vec{r}, \vec{\Omega})$, then it is more efficient to solve for the importance function $\psi_g(\vec{r}, \vec{\Omega})$ and perform the convolution indicated by the second part of equation (A33). However, if the value of the functional is needed for a number of different interaction cross sections $P_g(\vec{r}, \vec{\Omega})$, then it is more efficient to solve for the fluxes $\phi_g(\vec{r}, \vec{\Omega})$ and perform the convolution indicated by the first part of equation (A33).

In the perturbed reactor the functional giving the contributions caused by the given physical process for the neutrons in the system is, in analogy to equation (A14), equal to

$$F^p = \sum_g \int_{\vec{\Omega}} \int_R \mathscr{F}_g(\vec{r}, \vec{\Omega}) P_g^p(\vec{r}, \vec{\Omega}) \, d\vec{r} d\Omega \qquad (A36)$$

Here the general case of a perturbed system is considered for which $P_g^p(\vec{r}, \vec{\Omega})$ is the perturbed value of the cross-section-like quantity $P_g(\vec{r}, \vec{\Omega})$. The quantity $P_g^p(\vec{r}, \vec{\Omega})$ is taken to be

$$P_g^p(\vec{r}, \vec{\Omega}) = P_g(\vec{r}, \vec{\Omega}) + \delta P_g(\vec{r}, \vec{\Omega}) \qquad (A37)$$

where $\delta P_g(\vec{r}, \vec{\Omega})$ represents the perturbation in the interaction cross sections $P_g(\vec{r}, \vec{\Omega})$.

Next consider the difference $\delta F$ of the functionals $F^p$ and F. Eliminate the first term of equation (A30) by using the boundary conditions given by equations (A24) and (A32). Then insert equations (A33) and (A36) into equation (A30) giving the following result:

$$4\pi\delta F = 4\pi F^p - 4\pi F$$

$$= -4\pi \cdot \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\; \delta\sigma_g(\vec{r})\psi_g(\vec{r},\vec{\Omega})\mathscr{F}_g(\vec{r},\vec{\Omega})$$

$$+ \sum_{l=0}^{\infty} (2l+1) \cdot \sum_{m=-l}^{l} \int_R dr \sum_{g'} \mathscr{F}_{l,m}^{g'}(r) \cdot \sum_g \delta\sigma_{es}^l(r, g'\to g)\psi_{l,m}^g(r)$$

$$+ \int_R d\vec{r} \sum_{g'} \mathscr{F}_{g'}(\vec{r}) \cdot \sum_g \delta\sigma_{in}(\vec{r}, g'\to g)\Psi_g(\vec{r}) + \int_R d\vec{r} \sum_{g'} \mathscr{F}_{g'}(\vec{r}) \cdot \sum_g \delta\sigma_{n2n}(\vec{r}, g'\to g)\Psi_g(\vec{r})$$

$$+ 4\pi \cdot \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\; \psi_g(\vec{r},\vec{\Omega})\delta Q_g(\vec{r},\vec{\Omega}) + 4\pi \cdot \sum_g \int_{\vec{\Omega}} d\Omega \int_R d\vec{r}\; \mathscr{F}_g(\vec{r},\vec{\Omega})\delta P_g(\vec{r},\vec{\Omega}) \quad (A38)$$

Equation (A38) is the desired perturbation expression for a system with fixed sources. This equation gives the change in the functional F for a given physical process as a result of changes in various neutron cross sections, changes in the fixed source, and changes in the interaction process itself. The third term on the left side of equation (A30) has been split into its component parts comprising elastic scattering, inelastic scattering, and the (n, 2n) reaction. The elastic scattering reaction is considered to be anisotropic, with $\delta\sigma_{es}^l(g'\to g)$ being the perturbed values of the $l^{th}$-order macroscopic transfer cross sections. Inelastic neutron scattering and the (n, 2n) reaction are considered to be isotropic in the laboratory coordinate system with $\delta\sigma_{in}(g'\to g)$ and $\delta\sigma_{n2n}(g'\to g)$ being the perturbed values of the macroscopic inelastic scattering and (n, 2n) cross sections, respectively.

Equation (A38) is an exact relationship since no approximations are inherent in its derivation. However, since only low-order perturbation theory is being considered, the perturbed flux $\mathscr{F}_g(\vec{r},\vec{\Omega})$ can be replaced by its unperturbed value, $\phi_g(\vec{r},\vec{\Omega})$.

## Efficiency Function for Functional F

Definition of efficiency function. - Abagyan et al. introduce in reference 8 the concept of a material efficiency function $h^q(\vec{r})$ relative to a functional F:

$$h^q(\vec{r}) = \frac{4\pi\delta F^q(\vec{r})}{\delta\rho^q(\vec{r})} \quad (A39)$$

The efficiency function defines the change in a functional $F$ caused by the introduction of a unit quantity of material $q$ at the point $\vec{r}$. The efficiency function shows the sensitivity of the physical process to changes in the density of the different materials in the system. As can be seen, the quantity $h^q(\vec{r})$ has the dimension of the change in the functional per gram at position $\vec{r}$ for material $q$.

If the efficiency functions $h^q(\vec{r})$ are known, then the variation of the functional $\delta F^q$ with the change of density of material $q$ in a unit volume at position $\vec{r}$ by a value $\delta\rho^q(\vec{r})$ is equal to

$$4\pi\delta F^q(\vec{r}) = h^q(\vec{r})\delta\rho^q(\vec{r}) \tag{A40}$$

and

$$4\pi\delta F^q = \int_R h^q(\vec{r})\delta\rho^q(\vec{r})\,d\vec{r} \tag{A41}$$

$$4\pi\delta F = \sum_q 4\pi\delta F^q \tag{A42}$$

Thus, a knowledge of efficiency functions provides information about changes in functionals resulting from small changes in material densities $\delta\rho^q(\vec{r})$. The efficiency functions $h^q(\vec{r})$ can be calculated by means of the perturbation expression given by equation (A38).

Equation (A38) is the basic equation for the computation of the changes in the functional $F$ due to changes in the cross sections. Some of the terms in equation (A38) can be put in terms of efficiency functions as defined by equation (A39), as will be shown in the next sections which follow, with the perturbed fluxes replaced by their unperturbed values.

Efficiency function for total-cross-section term. - Let the change in the functional $F$ due to changes in the total cross section for material $q$ (the first term on the right side of eq. (A38)) be designated as $\delta F_t^q$. That is, let

$$4\pi\delta F_t^q = -4\pi\cdot\sum_g \int_{\overline{\Omega}} d\Omega \int_R d\vec{r}\,\delta\sigma_g^q(\vec{r})\psi_g(\vec{r},\vec{\Omega})\phi_g(\vec{r},\vec{\Omega}) \tag{A43}$$

The integration over $\vec{\Omega}$ in equation (A43) can be easily performed by using equations (A2) and (A25) along with the equation for the orthogonality property of the spherical

harmonics, equation (A7). This will give for $\delta F_t^q$ the following expression:

$$4\pi\delta F_t^q = -\sum_g \int_R d\vec{r}\, \delta\sigma_g^q(\vec{r}) \cdot \sum_{l=0}^{\infty} (2l+1) \cdot \sum_{m=-l}^{l} \phi_{l,m}^g(\vec{r})\psi_{l,m}^g(\vec{r}) \qquad (A44)$$

The quantity $\delta\sigma_g^q$ is the change in the macroscopic total cross section $\sigma_g^q$ for material q due to changes in the density of material q or to changes in the cross section itself. In other words, $\delta\sigma_g^q$ is equal to

$$\delta\sigma_g^q(\vec{r}) = \frac{\delta\rho^q(\vec{r})N_{av}}{A^q}\mu_{t,g}^q + N_o^q(\vec{r})\,\delta\mu_{t,g}^q \qquad (A45)$$

where $\mu_{t,g}^q$ is the microscopic total cross section for group g for material component q. The quantity $A^q$ is the atomic weight for material q, $N_{av}$ is the Avogadro number, and $N_o^q(\vec{r})$ is the original atom density of material q at position $\vec{r}$. The quantity $\delta\mu_{t,g}^q$ may be, for example, the estimated experimental error in the total cross section for group g for material q. The quantity $\delta\rho^q(\vec{r})$ represents the change in the density of material q at position $\vec{r}$.

Let us write equation (A43) in the following form:

$$4\pi\delta F_t^q = 4\pi\delta F_t^q(\rho) + 4\pi\delta F_t^q(XS) \qquad (A46)$$

That is, we wish to consider $\delta F_t^q(\rho)$ as the change in the functional $\delta F_t^q$ due to a change in the density of material q and to consider $\delta F_t^q(XS)$ as the change in the functional due to changes in the group-dependent microscopic-cross-section data. Thus, $4\pi\delta F_t^q(\rho)$ is given by

$$4\pi\delta F_t^q(\rho) = \int_R h_t^q(\vec{r})\delta\rho^q(\vec{r})\,d\vec{r} \qquad (A47)$$

with the efficiency function $h_t^q(\vec{r})$ being equal to

$$h_t^q(\vec{r}) = -\frac{N_{av}}{A^q} \cdot \sum_g \mu_{t,g}^q \cdot \sum_{l=0}^{\infty} (2l+1) \cdot \sum_{m=-l}^{l} \phi_{l,m}^g(\vec{r})\psi_{l,m}^g(\vec{r}) \qquad (A48)$$

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The efficiency function $h_t^q(\vec{r})$ is defined here as the change in the functional F caused by a unit change in the density of material q at position $\vec{r}$ for the effect due to the total cross section. The component parts of the efficiency function given by equation (A48) as a result of absorption, elastic scattering, inelastic scattering, and (n, 2n) reactions may be obtained by using the appropriate partial cross section in place of the total cross section.

The quantity $\delta F_t^q(XS)$ is the change in the functional due to changes in the total cross section itself and is given by

$$4\pi\delta F_t^q(XS) = \int_R d\vec{r}\left\{-N_0^q(\vec{r})\cdot\sum_g \delta\mu_{t,g}^q \cdot \sum_{l=0}^{\infty}(2l+1)\cdot\sum_{m=-l}^{l}\phi_{l,m}^g(\vec{r})\psi_{l,m}^g(\vec{r})\right\}$$

(A49)

As indicated previously, the effect on the functional F of the partial cross sections which make up the total cross section can be computed by using equation (A49) with the appropriate cross section in place of the total cross section.

Efficiency function for elastic scattering transfer terms. - Let the change in the functional F due to changes in the elastic scattering transfer cross sections for material q (the second term on the right side of eq. (A38)) be designated by $\delta F_{es}^q$. Then this quantity is equal to

$$4\pi\delta F_{es}^q = \sum_{l=0}^{\infty}(2l+1)\cdot\sum_{m=-l}^{l}\int_R d\vec{r}\sum_{g'}\phi_{l,m}^{g'}(\vec{r})\cdot\sum_g \delta\Sigma_{es,q}^l(\vec{r},g'\to g)\psi_{l,m}^g(\vec{r})$$

(A50)

The quantity $\delta\Sigma_{es,q}^l(\vec{r},g'\to g)$ is the change in the macroscopic $l^{th}$-order elastic scattering transfer cross section for group g' to group g for material q due to changes in the density of material q or to changes in the transfer cross section itself. In other words,

$$\delta\Sigma_{es,q}^l(\vec{r},g'\to g) = \frac{\delta\rho^q(\vec{r})N_{av}}{A^q}\cdot\mu_{es,q}^l(g'\to g) + N_0^q(\vec{r})\delta\mu_{es,q}^l(g'\to g)$$

(A51)

where $\mu_{es,q}^l(g'\to g)$ is the microscopic $l^{th}$-order elastic scattering transfer cross section for group g' to group g for material component q. The quantity $\delta\mu_{es,q}^l(g'\to g)$ may be associated with, for example, experimental errors in the elastic scattering transfer cross sections.

Let us write equation (A50) in the following way,

$$4\pi\delta F_{es}^q = 4\pi\delta F_{es}^q(\rho) + 4\pi\delta F_{es}^q(XS) \tag{A52}$$

That is, we wish to consider $\delta F_{es}^q(\rho)$ as the change in the functional $\delta F_{es}^q$ due to a change in the density of material $q$ and to consider $\delta F_{es}^q(XS)$ as the change in the functional due to changes in the $l^{th}$-order microscopic elastic scattering transfer cross sections. Thus, $4\pi\delta F_{es}^q(\rho)$ is given by

$$4\pi\delta F_{es}^q(\rho) = \int_R h_{es}^q(\vec{r})\delta\rho^q(\vec{r})\,d\vec{r} \tag{A53}$$

with the efficiency function $h_{es}^q(\vec{r})$ being defined by

$$h_{es}^q(\vec{r}) = \frac{N_{av}}{A^q} \cdot \sum_{l=0}^{\infty}(2l+1)\cdot\sum_{m=-l}^{l}\sum_{g'}\phi_{l,m}^{g'}(\vec{r})\cdot\sum_{g}\mu_{es,q}^l(g'\to g)\psi_{l,m}^g(\vec{r}) \tag{A54}$$

The efficiency function $h_{es}^q(\vec{r})$ is defined here as the change in the functional $F$ caused by a unit change in the density of material $q$ at position $\vec{r}$ for the effect due to the elastic scattering transfer cross sections.

The quantity $\delta F_{es}^q(XS)$ is the change in the functional due to changes in the elastic scattering transfer cross sections and is equal to

$$4\pi\delta F_{es}^q(XS) = \sum_{l=0}^{\infty}(2l+1)\cdot\sum_{m=-l}^{l}\int_R d\vec{r}\left[N_o^q(\vec{r})\cdot\sum_{g'}\phi_{l,m}^{g'}(\vec{r})\cdot\sum_{g}\delta\mu_{es,q}^l(g'\to g)\,\psi_{l,m}^g(\vec{r})\right] \tag{A55}$$

Equations (A50) to (A55) also apply to inelastic scattering and the (n, 2n) reaction given by the third and fourth terms on the right side of equation (A38). All that needs to be done is to replace the elastic scattering transfer cross sections by appropriate inelastic scattering or (n, 2n) reaction transfer cross sections. Although the various scattering processes are split for convenience, we could combine all the scattering terms (elastic, inelastic, and (n, 2n)), which are second, third, and fourth terms of equation (A38). The result is equations (A54) and (A55) with $\mu_{es}^l(g'\to g)$ replaced by $\mu^l(g'\to g)$ - the total microscopic transfer cross section.

Efficiency function for the fixed source term. - Let the change in the functional $F$ due to changes in the fixed source term (fifth term on the right side of eq. (A38)) be designated by $\delta F_Q$. Then this quantity is equal to

$$4\pi\delta F_Q = 4\pi \sum_g \int_{\overline{\Omega}} d\Omega \int_R d\vec{r}\, \psi_g(\vec{r}, \vec{\Omega})\delta Q_g(\vec{r}, \vec{\Omega}) \tag{A56}$$

The quantity $\delta Q_g(\vec{r}, \vec{\Omega})$ represents the change in the fixed source for group g. Equation (A56) can be evaluated directly if values of $\delta Q_g(\vec{r}, \vec{\Omega})$ are known.

In computing the biological dose rate, if both the neutron and photon components of the dose rate must be computed, the following analysis is necessary (this does not apply to coupled neutron-gamma problems): Part of the photon dose rate is the result of gamma rays from radiative neutron capture and inelastic neutron scattering. This source term is assumed to be isotropic and is equal to

$$Q_g^q(r) = f_g^q Q^q(\vec{r}) \tag{A57}$$

where $Q^q(\vec{r})$ is given by

$$Q^q(r) = \sum_{g'=1}^{G_N} \sigma_{x,g'}^q(\vec{r})\Phi_{g'}(\vec{r}) \tag{A58}$$

In equation (A58), $Q^q(\vec{r})$ represents the process rate per cubic centimeter for material q at position $\vec{r}$ for a reaction with cross section $\sigma_{x,g}$ for neutron energy group g. The summation extends over all neutron energy groups. The quantity $f_g^q$ is the number of photons which appear in gamma group g for each reaction which occurs for material q.

The quantity $\delta Q_g^q(\vec{r})$ now represents a change in the secondary gamma source $Q_g^q(\vec{r})$ due to changes in the density of material q and the reaction cross sections $\sigma_{x,g}^q$. Thus, $\delta Q_g^q(\vec{r})$ is equal to

$$\delta Q_g^q(\vec{r}) = \delta\left\{f_g^q Q^q(\vec{r})\right\} = \delta f_g^q \cdot Q^q(\vec{r}) + f_g^q \cdot \frac{\delta\rho^q(\vec{r})}{\rho^q(\vec{r})} \cdot Q^q(\vec{r}) + f_g^q \cdot \sum_{g'=1}^{G_N} \sigma_{x,g'}^q(\vec{r})\delta\Phi_{g'}(\vec{r})$$

$$+ f_g^q N_o^q(\vec{r}) \cdot \sum_{g'=1}^{G_N} \delta\mu_{x,g'}^q \cdot \Phi_{g'}(\vec{r}) \tag{A59}$$

Equation (A59) is obtained by using equation (A58) and an equation analogous to equation (A45) for $\delta\sigma_{x,g}^q(\vec{r})$. In equation (A59), $\delta f_g^q$ is the change in the number of photons which appear in gamma group g for each reaction which occurs for material q. The

quantity $\delta\mu_{x,g}^q$ is the change in the microscopic reaction cross section for neutron energy group g for material q. The quantity $\delta\Phi_g(\vec{r})$ is the perturbation in the flux and is equal to $\mathscr{F}_g(\vec{r}) - \Phi_g(\vec{r})$.

Let us write equation (A56) for a given material q in the following way:

$$4\pi\delta F_Q^q = 4\pi\delta F_Q^q(\rho) + 4\pi\delta F_Q^q(XS) \tag{A60}$$

That is, we wish to consider $\delta F_Q^q(\rho)$ as the change in the functional $\delta F_Q^q$ due to a change in the density of material q and to consider $\delta F_Q^q(XS)$ as the change in the functional due to changes in the reaction cross sections and gamma spectra for the particular reaction which produces the secondary photon source. Thus, $4\pi\delta F_Q^q(\rho)$ is given by

$$4\pi\delta F_Q^q(\rho) = \int_R h_Q^q(\vec{r})\delta\rho^q(\vec{r})\,d\vec{r}$$

$$= \int_R d\vec{r}\left\{\sum_g f_g^q \Psi_g(\vec{r})\right\} \cdot \left\{\frac{\delta\rho(\vec{r})}{\rho(\vec{r})} \cdot Q^q(\vec{r}) + \sum_{g'=1}^{G_N} \sigma_{x,g'}(\vec{r}) \cdot \delta\Phi_{g'}(\vec{r})\right\} \tag{A61}$$

with the efficiency function $h_Q^q(\vec{r})$ being equal to

$$h_Q^q(\vec{r}) = \left\{\frac{Q^q(\vec{r})}{\rho(\vec{r})} + \frac{1}{\delta\rho} \cdot \sum_{g'=1}^{G_N} \sigma_{x,g'}^q(\vec{r}) \cdot \delta\Phi_{g'}(\vec{r})\right\} \cdot \sum_g f_g^q \Psi_g(\vec{r}) \tag{A62}$$

The efficiency function $h_Q^q(\vec{r})$ is defined here as the change in the functional F caused by a unit change in the density of material q at position $\vec{r}$ resulting from a change in the secondary source $Q^q(\vec{r})$.

The quantity $\delta F_Q^q(XS)$ is the change in the functional due to cross-section changes and is given by

$$4\pi\delta F_Q^q(XS) = \int_R d\vec{r}\left[\sum_g \delta f_g^q \Psi_g(\vec{r})\right] \cdot Q^q(\vec{r})$$

$$+ \int_R d\vec{r}\left[\sum_g f_g^q \Psi_g(\vec{r})\right] \cdot \left[N_o^q(\vec{r}) \cdot \sum_{g'=1}^{G_N} \delta\mu_{x,g'}^q \cdot \Phi_{g'}(\vec{r})\right] \tag{A63}$$

Total efficiency function for a material. - The total efficiency function $h_T^q(\vec{r})$ for a material $q$ is the sum of the efficiency functions derived in the preceding sections for various terms of equation (A38), that is,

$$h_T^q(\vec{r}) = h_t^q(\vec{r}) + h_{es}^q(\vec{r}) + h_{in}^q(\vec{r}) + h_{n2n}^q(\vec{r}) \tag{A64}$$

The efficiency function $h_T^q(\vec{r})$ is, therefore, the total change in the functional $F$ per gram of material $q$ introduced at position $\vec{r}$. The total dose functional $\delta F_T^q(\rho)$ caused by a change in the density of material $q$ is equal to

$$4\pi \delta F_T^q(\rho) = \int_R h_T^q(\vec{r}) \delta \rho^q(\vec{r}) \, d\vec{r} \tag{A65}$$

or equivalently,

$$\delta F_T^q(\rho) = \delta F_t^q(\rho) + \delta F_{es}^q(\rho) + \delta F_{in}^q(\rho) + \delta F_{n2n}^q(\rho) \tag{A66}$$

## Perturbation Equation for Functional F in Terms of Various Partial Functionals

The total change in the functional $F$ for a system with a fixed source is given by equation (A38). The preceding analysis has described the use of efficiency functions to calculate changes in the functional due to the density changes in the material components of the system. The change in the functional $F$ due to changes in the cross sections $\delta F_T^q(XS)$ of material $q$ is given by

$$\delta F_T^q(XS) = \delta F_t^q(XS) + \delta F_{es}^q(XS) + \delta F_{in}^q(XS) + \delta F_{n2n}^q(XS) \tag{A67}$$

Finally, equation (A38) can be evaluated in terms of equations (A56), (A66), and (A67). The result is

$$4\pi \delta F = \sum_q 4\pi \delta F_T^q(\rho) + \sum_q 4\pi \delta F_T^q(XS) + 4\pi \delta F_Q + 4\pi \delta F_P \tag{A68}$$

where $\delta F_P$ is defined by the equation

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$$4\pi\delta F_P = 4\pi \cdot \sum_g \int_{\overline{\Omega}} d\vec{\Omega} \int_R d\vec{r}\, \phi_g(\vec{r},\vec{\Omega})\delta P_g(\vec{r},\vec{\Omega}) \qquad (A69)$$

The summations in equation (A68) are over all material components $q$.

## Calculational Procedure

The calculational procedure for using perturbation theory for systems with fixed sources is as follows:

(1) Solve equation (A1), by using the boundary condition given by equation (A32), for the neutron fluxes using the given fixed source terms.

(2) Solve equation (A23), by using the boundary condition given by equation (A24), for the importances for the interaction process of interest.

(3) Compute the functional $F$ for the interaction process of interest by using equation (A14).

(4) Compute the functional $F$ by using equation (A33). The two values of this functional, computed by using equations (A14) and (A33), must be equal and represent a necessary condition on the solutions obtained for the fluxes and importances.

(5) Compute the change in the functional $4\pi\delta F$ for the physical process of interest due to perturbations in the cross sections, perturbations in the fixed source, and perturbations in the interaction process itself by using equation (A38).

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