COMPUTER CODE ANISN MULTIPLYING MEDIA AND SHIELDING CALCULATION I. THEORY

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1. INTRODUCTION

ANISN is a code originaly developed by Oak Ridge Computing Technology Center and Oak Ridge National Laboratory /1/, to solve the one-dimensional linear particle transport equation, also known as linear Boltzmann transport equation, in plane, spherical, or cylindrical geometry. The solution technique is an advanced discrete ordinates method, which is a generalization of the method used early in radiative transfer, by Wick /2/ and Chandrasekhar /3/, and by Carlson /4/ in neutron transport theory.

Since the Linear Boltzmann Transport equation is the basic physical model to describe the transport of uncharged particles such as neutrons and photons (γ rays, light etc), it is possible to use the ANISN code to solve shielding problems, including deep penetration and neutron-gamma coupled problems, as well as multiplying media problems in reactor theory, like cell calculation problems, criticality search and others.

Although there are several text books describing the transport theory and discrete ordinates method, such as Duderstadt & Martim /5/; Bell & Glasstone /6/; Willians/7/ and B. Davidson /8/, as well as several review papers, as those published by Stevens /9/; Sanches & McCormick /10/, and scientific reports, as those of Lee /11/; Lathrop/12/; here we wish to review briefly the transport equation and its solution methods, with an emphasis to the discrete ordinates method, in order to make the code more understandable, and not only used as a "black-box".

2. TRANSPORT EQUATION AND ITS SOLUTION METHOD

Transport Theory is the branch of physics devoted to study the evolution of the particle distribution function in the phase-space (space $\underline{r}$; direction $\underline{\Omega}$; energy E), and it was first introduced in the kinetic theory, by Boltzmann (1872). The Boltzmann equations in their general form are a set of non-linear integro-differential equations, but assumptions such as: i) neglecting collisions between identical particles; ii) one type of particle being transported in a host medium; iii) classical particles; iv) density of transported particles orders of magnitude smaller than the density of the host medium, etc, make it possible to reduce these equations to one single linear, integro-differential equation describing the transported particle distribution function. The assumptions used to linearize the Boltzmann equation are adequate to describe the transport of uncharged particles, such as neutrons and photons, and the motion of molecules in a rarefied medium. Thus, the linearized Boltzmann equation is the basic equation in neutron transport theory in multiplying media, with application in the design of nuclear reactors and criticality analysis; in the theory of radiative transfer, with application in radiative heat transfer and calculations of stellar and planetary atmospheres; and in radiation shielding.

Although the linear Boltzmann equation can be derived from first principles of physics, it is more easily obtained by a simple balancing of the various mechanisms by which particles can be gained or lost from an element in a phase-space, $(\underline{r},\underline{\Omega},E)$, i.e;

$$\begin{bmatrix}\text{time rate of}\\ \text{particle density}\\ \text{change}\end{bmatrix} = \underset{(I)}{\begin{bmatrix}\text{change due}\\ \text{physical}\\ \text{leakages}\end{bmatrix}} + \underset{(II)}{\begin{bmatrix}\text{change due}\\ \text{to}\\ \text{collisions}\end{bmatrix}} + \underset{(III)}{\begin{bmatrix}\text{sources}\end{bmatrix}},$$

and this balance condition can be expressed mathematically as

$$\frac{1}{v}\frac{\partial}{\partial t}\Phi(\underline{r},\underline{\Omega},E;t) = \underset{(I)}{-\underline{\Omega}.\nabla\Phi(\underline{r},\underline{\Omega},E;t)} + \underset{(III)}{S(\underline{r},E,\underline{\Omega},t)}$$

$$\underset{(II)}{-\Sigma_t(\underline{r},E,t)\Phi(\underline{r},\underline{\Omega};E;t) + \int_0^\infty dE'\int_{4\pi} d\Omega'\Sigma(\underline{r};E'\rightarrow E;\underline{\Omega}'.\underline{\Omega};t)\Phi(\underline{r},\Omega',E',t)}, \qquad (1)$$

where $\Phi(\underline{r},\underline{\Omega},E,t)$ is the angular flux, or angular particle track length; $\Sigma_t(\underline{r},E,t)$ is the total macroscopic cross section; $\Sigma(r,E'\rightarrow E,\Omega.\underline{\Omega}';t)$ is the differential transfer cross section, describing the probability that a particle with an initial energy E' and direction $\underline{\Omega}'$ undergoes a collision at $\underline{r}$ in a time t, resulting in a change of direction and energy; and $S(\underline{r},\Omega,E,t)$ is the source-term.

Equation (1) can be applied for neutrons or photons, depending on the correct physical interpretation of the interaction between the particle and the host medium (cross section).

For neutrons, besides a scattering reaction, a collision of neutrons with a host medium can generate other neutrons by fission (multiplying medium) and so the transfer kernel may include a term like.

$$\frac{\chi(E)}{4\pi}\int_0^\infty dE'\int_{4\pi} d\underline{\Omega}'\nu(E')\Sigma_f(\underline{r},E',t)\Phi(\underline{r},E',\underline{\Omega}',t), \qquad (2)$$

where $\chi(E)$ is the energy distribution of fission neutrons (spectrum); $\nu(E')$ is the average number of neutrons released per fission and $\Sigma_f(\underline{r},E';t)$ is the macroscopic fission cross section, assumed to be isotropic.

Usually, for practical applications, eq. (1) is solved in steady-state. Also, in case of multiplying media, it is to be expected that systems containing fissile nuclides can be regarded as being either subcritical, critical, or super critical. The criticality problem can often be best approached by introducing the effective multiplication factor (K_{eff}), to balance the fission source with others terms in the transport equation, in a manner such that the resulting system is critical (time-independent)*, i.e.

$$\underline{\Omega}.\nabla\Phi + \Sigma\Phi = \int_0^\infty\int_{4\pi}\Sigma_s(\underline{r},\underline{\Omega}'\to\underline{\Omega};E'\to E)\ \Phi(\underline{r},\underline{\Omega}',E')d\underline{\Omega}'dE'$$

$$+\frac{1}{K_{eff}}\int_0^\infty\int_{4\pi}\frac{\chi(E)}{4\pi}\ \nu(E')\Sigma_f(\underline{r},E')\Phi(\underline{r},E',\underline{\Omega}')d\underline{\Omega}'dE', \qquad (3)$$

The scattering kernel depends on the physical interaction, and usually, the angular dependence is expanded in Legendre polynomials of the scattering angle ($\underline{\Omega}.\underline{\Omega}'=\mu_0$); i.e,

*Physically, this can be understood from the fact that any system containing fissile material could be made critical by varying the number of neutrons emitted per fission from the original value (ν) to (ν/k).

$$\Sigma_s(\underline{r},E'\to E,\mu_0) = \sum_{\ell=0}^{L}\frac{2\ell+1}{2}\Sigma_s^{(\ell)}(\underline{r},E'\to E)P_\ell(\mu_0). \qquad (4)$$

The energy dependence is treated by a multigroup model, in which the energy range is divided into a finite number, G, of intervals separed by the energies E_g, g=1,2,3,...,G. Thus, the multigroup transport equation with anisotropic scattering, is written as:

$$\underline{\Omega}.\nabla\Phi_g(\underline{r},\underline{\Omega})+\Sigma_{tg}\Phi_g(\underline{r},\underline{\Omega}) = \sum_{m=0}^{M}\sum_{g'}^{G}\int_{4\pi}d\underline{\Omega}'\left(\frac{2\ell+1}{2}\right)\Sigma^{(\ell)}_{g'\to g}(\underline{r})\,P_\ell(\mu_0)\Phi_{g'}(\underline{r},\underline{\Omega}')$$

$$+\frac{\chi_g}{K_{eff}}\sum_{g'}^{G}\left(\frac{\nu\Sigma_f}{4\pi}\right)_{g'}\Phi_{g'}(\underline{r}) + S^g_{ext}(\underline{r});\ g=1,2,\dots,G, \qquad (5)$$

where, $\Phi_g(\underline{r},\Omega)$ is the group angular flux,

$$\Phi_g(\underline{r},\underline{\Omega}) = \int_{E_g}^{E_{g+1}}\Phi(\underline{r},E,\Omega)dE; \qquad (6)$$

and $\Phi_g = \int_\Omega \Phi_g d\Omega$ is the total flux. The group cross sections, or group constants, (Σ_{tg}; $\Sigma^{(\ell)}_{g'\to g}$; χ_g; $(\nu\Sigma_f)_g$) are flux weighted cross sections averaged over the group energy interval*, i.e.

$$\Sigma_g(\underline{r}) = \frac{\int_g\Sigma(r,E)\Phi(r,E)dE}{\Phi_g(\underline{r})}, \qquad (7)$$

* It is important to observe that the knowledge of the group constants that appear in these equations depends on the knowledge of the group fluxes which are not know before solving the transport equation for the problem. To overcome this difficulty, it is used as weighting function $\Phi(\underline{r},E)$ in equation(7), the approximate solution provided by the slowing-down or thermalization theory(in case of neutrons) or assume a flat flux(in case of gammas).The pointwise cross sections, needed to evaluate the group cross section, is given from Nuclear data libraries, such as "Evaluated Nuclear Data File"(ENDF).

and

$$\Sigma^{(\ell)}_{g'\to g}(\underline{r}) = \frac{\int_g dE \int_{g'} \Sigma^{(\ell)}(\underline{r},E'\to E) \int_{4\pi} \Phi(\underline{r},E',\underline{\Omega}')\, P_\ell(\mu_o)\, dE'\, d\Omega'}{\int_{g'} \int_{4\pi} \Phi(\underline{r},E',\underline{\Omega}')\, P_\ell(\mu_o)\, d\Omega'\, dE'} \; ; \quad (8)$$

The determination of the group constant involves two stages, First, the cross section variation with energy must be available, and second an approximation for the flux must be made (energy spectrum). This is accomplished by performing a set of auxiliary calculations, in a very specific field, whose details are beyond the scope of this text. There are several code systems which can be used to generate the group constants, from well known data libraries (ENDF, ENDL, VITAMIN C etc). An example of such system is AMPX /13/, which generates neutron, gamma or coupled neutron-gamma multigroup cross sections from basic data of ENDF/B (Evaluated Nuclear Data File).

An outline of the neutron multigroup calculation usually carried out by most of the nuclear codes is illustrated by the block diagram in figure 1. For gamma, or neutron-gamma coupled systems (shielding problems), there is nothing like criticality search, and there is only downscattering (fixed source problem). To couple neutron and gammas, the equations (5) are divided into two sets, an upper set consisting of N-groups of neutrons ($g=1,2,\ldots,N$), and a lower set consisting of G-groups of gammas ($g = N+1, N+2, \ldots, N+G$), and these two sets coupled by a transfer cross section ($\Sigma_{n\to g}$) due to nuclear reactions with neutrons producing gammas, such as capture, or inelastic scattering reactions.

The steady-state linear transport equation applied to physical problems is a typical boundary value problem, and to obtain a unique (and positive) solution it is necessary to have the boundary conditions well defined, which

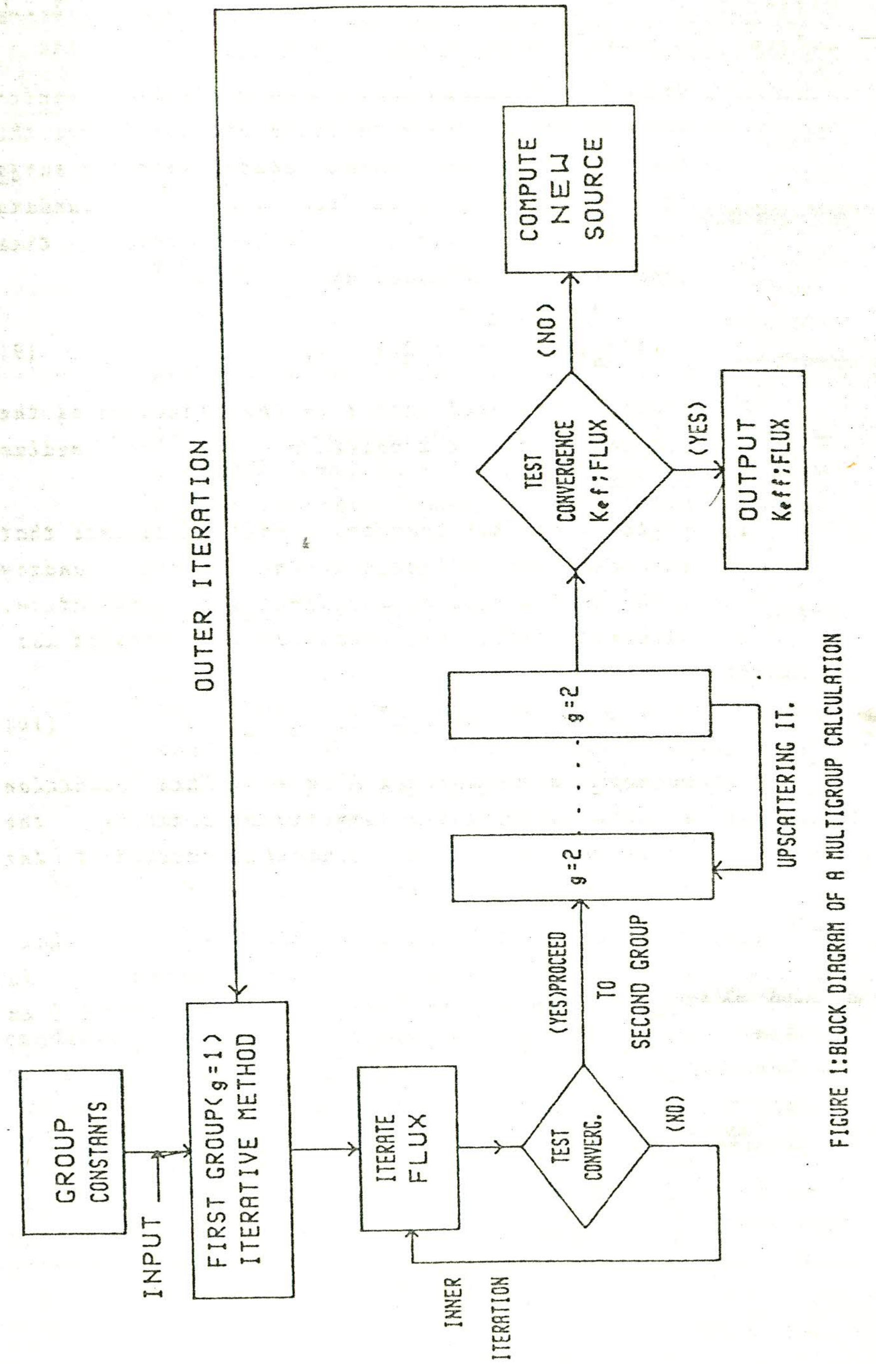


FIGURE 1:BLOCK DIAGRAM OF A MULTIGROUP CALCULATION

establish the physical conditions of the problem being solved. The most commonly used boundary conditions are :

i) Vacuum or Free Surface: If no particles enter the medium, and if a particle once it leaves the the medium surface cannot return, then the surface is called a free surface, and the boundary condition is vacuum type. Mathematically, this condition is expressed as

$$\Phi(\underline{r}_s,\underline{\Omega},\ E) = 0;\ \underline{\Omega}.\underline{n} < 0, \quad (9)$$

where $\underline{n}$ is a unit vector in the direction of the outward normal at a position $\underline{r}_s$ in the medium surface.

ii) Reflection: This boundary condition assumes that particles are reflected at the surface boundary with equal angles of incidence and reflection. Mathematically, this condition is expressed as;

$$\Phi(\underline{r}_s,\underline{\Omega},E) = \Phi(\underline{r}_s,\underline{\Omega}^*,E);\ \underline{\Omega}^*.\underline{n} < 0 \quad (10)$$

where $\underline{\Omega}^*.\underline{n} = -\underline{\Omega}.\underline{n};\ \underline{\Omega} \times \underline{\Omega}^*.\underline{n} = 0$. This condition is used to express a symmetry property of the solution, and is the one usually adopted at the outerboundary of unit cell calculation.

iii) Periodic: This boundary conditions assumes that the angular flux leaving certain boundary is equated with the re-enter in other boundary (in ANISN, angular flux leaving left-boundary re-enters in the right boundary).

iv) white: The angular flux leaving the specified boundary is integrated over the angular variable, and this total flux is then returned isotropically at the same boundary as function of energy and angles.

v) Albedo: in ANISN, this condition is interpreted as a generalization of the white boundary condition, and is obtained assuming that the isotropically returned angular flux is multiplied by the Albedo, i.e.,

$$\Phi(\underline{r}_s,\underline{\Omega},E) = \frac{\alpha}{4\pi} \int_{2\pi(\underline{\Omega}',n > 0)} \Phi(\underline{r}_s,\Omega',E)d\underline{\Omega}';\ \underline{\Omega}.n < 0, \quad (11)$$

where α is the Albedo $(0 < \alpha < 1)$

vi) Specified Incoming Angular Flux : this boundary condition specifies the incoming angular flux at the boundary (inhomogeneous boundary condi - tion), i.e.;

$$\Phi(\underline{r}_s,\underline{\Omega},E) = \Phi_{in}(\underline{\Omega},E);\ \underline{\Omega}.\underline{n} < 0, \quad (12)$$

where Φ_{in} is a know function of energy and angle. In ANISN this boundary condition is not available explicitly but it can be simulated using the option of shell source (or surface source), i.e, an incident flux may be replaced by an equivalent surface source,

$$S(\underline{r}_s,\underline{\Omega},E) = -\underline{n}.\underline{\Omega}\ \Phi_{in}\ (\underline{\Omega},E). \quad (13)$$

The solution of the transport equation under the boundary conditions is not an easy task, and deterministic methods can solve it only in regular geometries (the Monte-Carlo Method which is a stochastic way to solve the integral transport equation can be used in non-regular geometries).

The transport code ANISN solves the multigroup trans - port equation with anisotropic scattering in one- dimensional geometries (slab; cylindrical, or spherical), and in this case the transport equation is reduced to the forms illustrated in table 1 (one-group).

Exact solutions of the transport equation (closed form) can be obtained only for very idealized physical models, by the singular eigen function expansion method (or Case's Method), and the Fourier transform method. Excellent reviews of analytical solution of the transport equation are provided by the classical book of Case & Zweifel /14/, and by Mc Cormick & Kuscer /15/.

For practical problems, the solution of the transport equation is accomplished by numerical means. A large variety of numerical methods have been developed, which at first glance, appears quite different, however all these methods are based on a few approximation techniques, such as finite differences for differential operators; quadrature formulas for integral operators; or expansion methods. Among several methods the most used are : spherical harmonics expansion method (or P_N, or DP_N method); discrete ordinates (or S_N method); Finite Elements method; characteristic's method; Integral transport methods (collision probability; integral transform); interface or surface integral methods (C_N, F_N methods; invariant imbedding); and nodal or coarse mesh methods. A review of these methods is provide by Sanches & Mc Cormick /10/. Here, the discrete ordinates method is reviewed, since this is the method used by the ANISN code.

3. DISCRETE ORDINATES, OR S_N METHOD

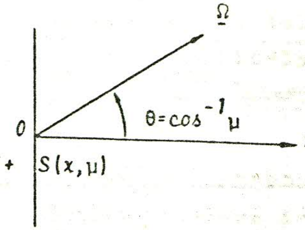
The original method of discrete ordinates is attributed to Wick /2/and Chandrasekhar /3/ which applied this method to solve plane geometry problems in Radiative Transfer. A generalization to spherical and cylindrical geometries was introduced by Carlson /4/, who introduced the name by which the method is know, S_N method*. Since then, this technique has been used by several codes in different versions, such as DTF; ANISN; DOT; XSDRN; TWOTRAN

Table 1: The form of Linear Transport Equation in one dimensional geometries (one group model)

Slab Geometry: $(x.\mu)$

$$\mu \frac{\partial}{\partial x} \psi(x,\mu) + \Sigma(x)\, \psi(x,\mu) =$$

$$\sum_{\ell=0}^{L} \frac{2\ell+1}{2}\, \Sigma_s^{(\ell)}(x)\, P_\ell(\mu) \int_{-1}^{1} \psi(x,\mu')P_\ell(\mu')d\mu' + S(x,\mu)$$



Obs: $S(x,\mu)$= external fixed source+fission

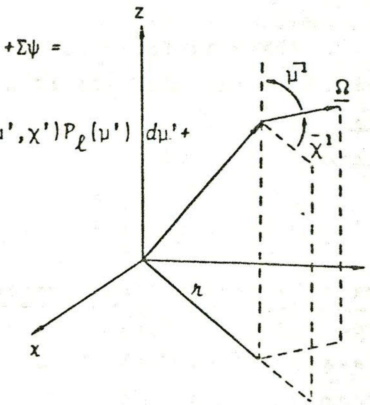
L = scattering order

Cylindrical Geometry: (r,μ,χ)

$$\sqrt{1-\mu^2}\, \cos\chi \frac{\partial}{\partial r}\psi - \frac{\sqrt{1-\mu^2}}{r} \sin\chi \frac{\partial}{\partial \chi}\psi + \Sigma\psi =$$

$$\sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi}\, \Sigma_s^{(\ell)}(r) P_\ell(\mu) \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\chi \psi(r,\mu',\chi')P_\ell(\mu')\, d\mu' +$$

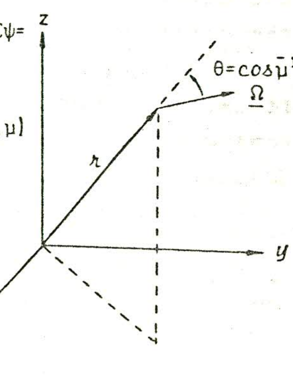
$$S(r,\mu,\chi)$$



Spherical Geometry: (r,μ)

$$\frac{\mu}{r^2} \frac{\partial}{\partial r}\left[r^2\psi(r,\mu)\right] + \frac{1}{r} \frac{\partial}{\partial \mu}\left[(1-\mu^2)\psi(r,\mu)\right] + \Sigma\psi =$$

$$\sum_{\ell=0}^{L} \frac{2\ell+1}{2}\, \Sigma_s^{(\ell)}(r) P_\ell(\mu) \int_{-1}^{L} \psi(r,\mu')P_\ell(\mu')d\mu' + S(r,\mu)$$



Obs: Conservative form of transp. eq.

etc. Several of these codes are available from Radiation Shielding Information Center (RSIC), in USA, and in N.E.A Data Bank, in Europa /16/. Table 2 illustrates a short list of the most popular codes using Discrete Ordinates method.

In the discrete ordinates method, the angular variable is discretized into a number of discrete directions (angular quadratures, with associated weights, to approximate integrals); the spatial variable is treated by a finite difference scheme, and the energy variable, by myltigroup method, i.e,

$$(\underline{r},\underline{\Omega},E) \xrightarrow[\text{Ordinates}]{\text{Discrete}} (\underline{r}_j;\underline{\Omega}_m;E_g)$$

The transport equation is discretized into a discrete phase-space cell, resulting in a system of algebraic equations at the discrete mesh points r_j ; Ω_m for each energy group, i.e,

$$\underline{\underline{A}}\ \underline{\Phi} = \underline{\underline{B}}\ \underline{\Phi} + \underline{\underline{S}}\ , \qquad (14)$$

where $\underline{\underline{A}}$ is a matrix representing the streaming-collision operator $(\underline{\Omega}.\nabla + \Sigma)$; $\underline{\underline{B}}$ is a matrix representing the group in-scattering term; $\underline{\underline{S}}$ is a matrix representing the source-term (external, plus group-to-group scattering sources, including fission), and $\underline{\Phi}$ is the angular flux vector at the discrete group mesh points. The numerical solution of the algebraic equations can be obtained by an interactive scheme, inner iteration, $(\underline{\Phi}^{(n)} = \underline{\underline{A}}^{-1}\underline{\underline{B}}\Phi^{(n-1)} + \underline{\underline{A}}^{-1}\underline{\underline{S}})$, using some acceleration method (coarse mesh rebalancing; linear diffusion synthetic etc).

The selection of the discrete ordinates quadrature set; Ω_m directions, and w_m weights to discretize the transport equation, by approximating integral angular terms;

$$\int_{\Omega} \Phi(\underline{r},\Omega)d\Omega \simeq \sum_{m=1} \Phi(\underline{r},\underline{\Omega}_m)\ w_m\ ,$$

* In the original version it was assumed that the angular fluxes varies with angle as if they were connected by Straight lines.

Table 2 - Discrete Ordinates, S_N, Codes

Name	Geometry	Comments
D T F (K.D. Lathrop,) W.W. Engle	One dimensional (plane; spherical, cylindrical)	Linear Anisotropic Scattering (P-1) Versions: DTF-II; DTF-IV; DTF-69 (LASL)
ANISN (W.W. Engle)	One dimensional (plane; spherical, cylindrical)	General Anisotropic Scattering Versions: ANISN-ORNL; ANISN-W; ANISN-E; ANISN-JR; ANISN-PC; ANISN-A (ORNL)
XSDRN (N.M. Greene; C.W. Craven; Jr.)	One dimensional (plane; spherical, cylindrical)	Performs group cross section averaging (cell calculation) Versions: XSDRNPM (ORNL)
D O T (F.R. Mynatt)	Two dimensional (X-Y; R-Z; R-Θ)	General Anisotropic Scattering Versions: DOT II; DOT III; DOT 3.5; DOT-2DB; DOT II-W; DOT-4.2; DORT (ORNL)
TWOTRAN (Lathrop)	Two dimensional (X-Y; R-Z; R-Θ)	General Anisotropic Scattering Versions: TWOTRAN-GG-FC; TWOTRAN-GG-VW; TWOTRAN-PNVW; TWOTRAN-V; TWOTRAN-SPHERE (LASL)
TRIDENT (Seed, Miller; Brinkley)	Two dimensional (X-Y; R-Z). Regular triangular mesh	General Anisotropic Scattering. Finite Element Versions: TRIDENT-CTR (LASL)
TORT (W.A. Rhoads & R.L. Childs)	Three dimensional (X-Y-Z)	(ORNL)
THREETRAN (K.D. Lathrop)	Three dimensional (X-Y-Z)	(LASL)

is basic to obtain an accurate numerical solution, and has been guided by two main principles: i) physical symmetry; and ii) the arrangement of discrete directions on latitudes on the unit sphere. A complete discussion on discrete ordinates angular quadratures is provided by Lathrop & Carlson /17/.

For one dimensional geometries, the following criteria must be satisfied by the quadrature set; μ_m ; w_m

i) invariance projection, i.e μ_m symmetric about $\mu=0$, or : $\mu_i = -\mu_{m+1-i}$, $w_i = w_{m+1-i}$ (symmetric uppon reflection).

For certain shielding calculations, the solution is forward peaked (concentrated near $\mu=1$), and so using a symmetric quadrature will not provide accurate solutions. In this case, a biaside quadrature set must be used

ii) positivity of the solution, i.e; $w_m>0$, $\sum_{m=1}^{M} w_m = 1$.

From (i), and (ii), the condition to be sastified is $\sum_{m=1}^{M} \mu_m w_m = 0$.

iii) Accurate evaluation of integrals. Gaussian quadrature set integrates exactly a polynomial of degree 2N-1, i.e,

$$\sum_{m=1}^{M} w_i \mu_i^N = \frac{2}{N+1} \; ; \; N \text{ even}$$
$$= 0 \; ; \; N \text{ odd}, \qquad (16)$$

and so, would be a good scheme to choose. However, ANISN code does not use Gaussian quadrature sheme, it rather uses a quadrature scheme which satisfies condition (i), and (ii), and in addition satisfies the "diffusion theory" condition /17/,

$$\sum_{m=1}^{M} w_m \mu_m^2 = \frac{1}{3} . \qquad (17)$$

In the manual /1/, a symmetric quadrature suggested to to be used in ANISN code is presented. From this set, we note that for plane or spherical geometries, S_N discrete quadrature requires (N+1) directions, and for cylindrical geometry (curved) it is required (N+4)N/4 directions. The code DOQDP-ADOQ (Discrete Ordinates Quadratures Generator), distributed by RSIC, or NEA-DB (PSR-0110) /18/, generate symmetric, or asymmetric discrete ordinates quadrature (direction cosines and weights) to be used by S_N codes (ANISN, DOT, and others).

Due to the angular discretization scheme, an undesirable effect occurs, the so called "ray effect, in which the finite number of rays used in a discrete ordinate representation miss localized sources, or absorber, producing deletetious numerical effects in the solution of the transport equation. For a discussion on the "ray effect", it is recommended the papers of Lathrop /19,20/.

To illustrate the main features of the Discrete Ordinate method, consider the one-group transport equation for slab geometry, with isotropic scattering (L=0), as given in table 1, and a discretization of the phase-space as shown in figure 2 (discrete spatial meshes $x_1, x_2, \ldots x_i$; and angular quadratures, $\mu_1, \mu_2, \ldots, \mu_m$), with associated weights $w_1, w_2, \ldots, w_m$). Thus, writting the transport equation for each discrete direction, μ_m; using a second order central difference discretization for the spatial variable; and approximating the scattering integral term by a quadrature formula, the discretized transport equations become,

$$\mu_m \left(\frac{\Phi_{m;i+1/2} - \Phi_{m;i-1/2}}{\Delta x_i} \right) + \Sigma_t^i \, \Phi_{m,i}$$
$$= Q_{m,i} \; ; \; i = 1,2,\ldots,I \quad m = 1,2,\ldots,M, \qquad (18)$$

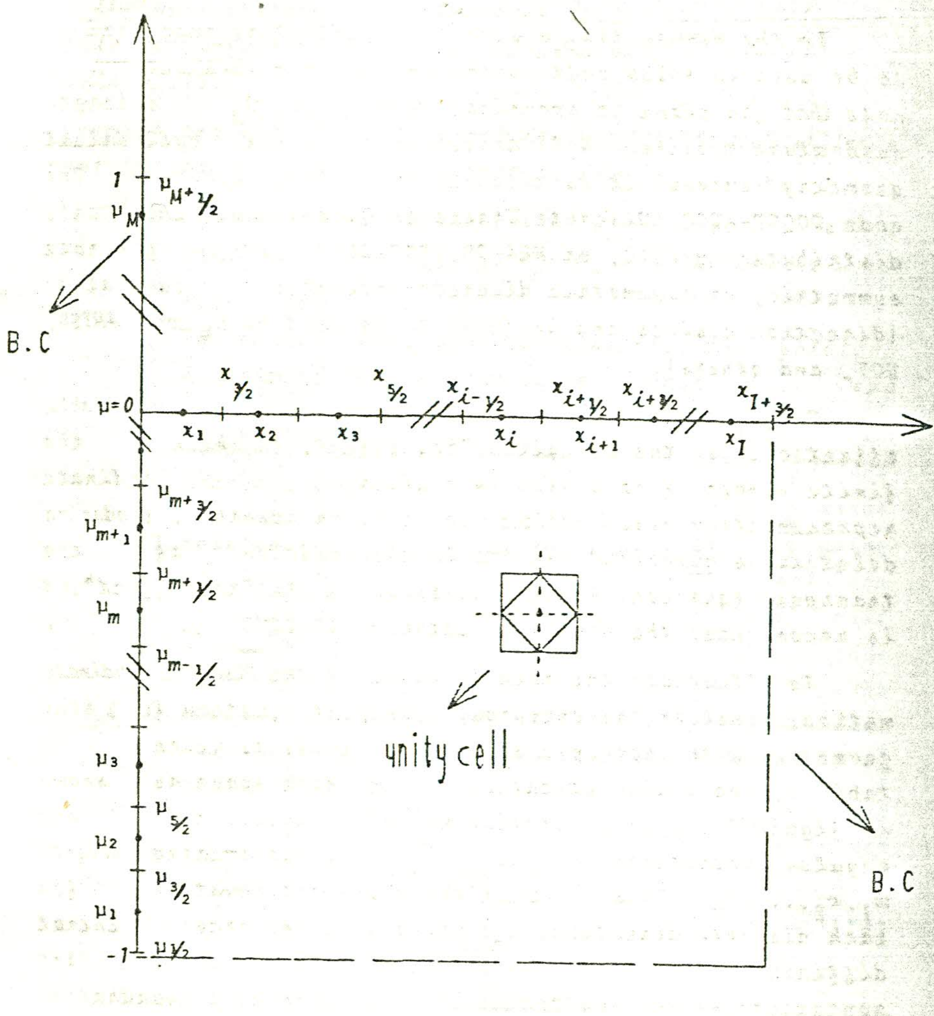


figure 2: discrete ordinates mesh points

where

$$Q_{m,i} = \frac{1}{2}\Sigma_s^i \sum_{m=1}^{M} w_m \Phi_{m,i} + S_{m,i}. \tag{19}$$

Due to the iterative method of solution, it is assumed that $Q_{m,i}$ is known, and this quantity is updated, at each new iteration (inner iteration). The boundary conditions, discussed before, assume that $\Phi_{m,1/2}$; $m = 1,2,\ldots,\frac{M}{2}$ (positive directions, $\mu>0$); and $\Phi_{m,I+1/2}$; $m = \frac{M}{2}\ldots,M$ (negative directions, $\mu<0$) are specified.

First, it is noted that there are IxM equations for (2I+1)xM unknowns ($\Phi_{m,i+1/2}$; $\Phi_{m,i-1/2}$; $\Phi_{m,i}$), and even using the M equations given by B.C., it is still not possible to solve equations (18). Therefore, it is necessary to obtain IxM more equations to solve the problem. These equations are obtained by relating the fluxes $\Phi_{m,i}$ to the half-node fluxes, $\Phi_{m,i\pm1/2}$, by :

$$\Phi_{m,i} = \frac{\Phi_{m,i+1/2} + \Phi_{m,i-1/2}}{2} \quad ; \quad i = 1,2,\ldots,I, \quad m = 1,2,\ldots,M. \tag{20}$$

Equations (20) are the one-dimensional version of the general scheme called "diamond difference". Therefore, substuting Eqs. (20) into Eqs (18), we obtain :

$$\Phi_{m,i+1/2} = \left(\frac{1-\Sigma_{t,i}\,\Delta X_i/2\mu_m}{1+\Sigma_{t,i}\,\Delta X_i/2\mu_m}\right)\Phi_{m,i-1/2} + \frac{Q_{m,i}}{\mu_m/\Delta X_i+\Sigma_{t,i/2}} ; \mu_m > 0, \tag{21}$$

and

$$\phi_{m,i-1/2} = \left(\frac{1-\Sigma_{t,i}\Delta X_i/2\mu_m}{1+\Sigma_{t,i}\Delta X_i/2\mu_m}\right)\phi_{m,i+1/2} + \frac{Q_{m,i}}{-\mu_m/\Delta X_i+\Sigma_{t,i}/2}; \quad \mu_m < 0. \qquad (22)$$

Equations (21), and (22) give a strategy to solve the transport equation, i.e, starting at the boundary $I+1/2$, where the angular flux $\phi_{m,I+1/2}$ is specified for $\mu_m < 0$, the solution advances for all values of $\mu_m < 0$ using equation (22). For $\mu_m > 0$, the boundary conditions specify the angular flux at $X_{1/2}$, and the solution advances for all values of $\mu_m > 0$ using equation (21).

The strategy used to construct the solution may give origen to numerical unstability, or negative fluxes. To see, how it may occur, we note that if equation (21) is used the solution is stable, since the error will advance with $(1-\Sigma_t\Delta X/2\mu_m)/(1+\Sigma_t\Delta X/2\mu_m)$, and since $\mu_m > 0$ the error will be dumped as the solution advance. However, using equation (22), the error may be amplified as the solution advances. To avoid unstability of the solution, care must be taken in the choice of the mesh length. In ANISN code there are some empirical prescriptions to avoid such unstability, as for example: The radial mesh should be, $\Delta R < (1+\Sigma_{g\to g}/\Sigma^t_g)/4\Sigma^t_g$, and the axial mesh $\Delta Z < 2/\Sigma^t_g$, where Σ^t_g is the largest total group cross section, and $\Sigma_{g\to g}$ is the within group scattering cross section for the selected group. Besides, this criteria should be applied near boundary region, or where large flux gradients may occur. Also, a mesh size should not vary more than a factor of two between adjacent mesh regions.

To guarantee the positivity of the solution, discrete ordinate codes, such as ANISN, have some "fixup" routines. These routines involve local modification of the difference scheme whenever a negative flux occurs, being one of the most used of such routines being "step scheme". In this scheme, the equations (20) are modified to,

$$\Phi_{m,i} = \alpha\Phi_{m,i+1/2} + (1-\alpha)\Phi_{m,i-1/2}; \quad \mu_m > 0, \qquad (23)$$

$$\Phi_{m,i} = \alpha\Phi_{m,i-1/2} + (1-\alpha)\Phi_{m,i+1/2}; \quad \mu_m < 0, \qquad (24)$$

where for $\alpha = 1/2$, Eqs (23), (24) are reduced to the "diamond scheme", while choosing $\alpha = 1$ (step model) the positivity of the solution will be guaranted, although with some lost of accuracy.

The derivation used in the plane geometry discrete ordinates case is not used in curved geometries (spherical, or cylindrical). In this case, a conservative form of the transport equation is integrated in a discrete ordinate celi (see figure 2) to obtain a general discrete ordinates equation in one-dimensional geometry;

$$\mu_m(A_{i+1/2}\Phi_{m,i+1/2} - A_{i-1/2}\Phi_{m,i-1/2})$$

$$+ (a_{m+1/2}\Phi_{m+1/2,i} - a_{m-1/2}\Phi_{m-1/2,i})/w_m$$

$$+ \Sigma_{t,i}\Phi_{m,i}V_i = Q_{m,i}V_i; \quad i = 1,2,\ldots,I, \quad m = 1,2,\ldots,M, \qquad (25)$$

where area (A) and volume (V) elements for slab, spherical and cylindrical geometries are given in table 3, and the curvature coefficient, a, can be obtained by the recurrence relation,

$$a_{m+1/2} = a_{m-1/2} - \mu_m w_m(A_{i+1} - A_i), \qquad (26)$$

with $a_{1/2} = a_{m+1/2} = 0$. Of course, for plane geometry ($A=1$; $V_i = \Delta X_i$; $a_{m+1/2} = a_{m-1/2}$), eqs. (25) reduces to eqs. (18).

Table 3 - Area and Volume Elements for one-dimensional geometries.

	Plane	Spherical	Cylindrical
$A_{i\pm 1/2}$	1	$4\pi r^2_{i\pm 1/2}$	$2\pi r_{i\pm 1/2}$
V_i	ΔX_i	$4\pi r^2_i \Delta r_i$	$2\pi r_i \Delta r_i$

In solving equations (25), first we note that there are (3IM+I+M) unknowns for IM equations. Therefore, it is again necessary to relate the centered fluxes with the edges fluxes (see figure 2), i.e.,

$$\Phi_{m,i} = \alpha\Phi_{m,i+1/2} + (1-\alpha)\Phi_{m,i-1/2}, \qquad (27)$$

$$\Phi_{m,i} = \alpha\Phi_{m+1/2,i} + (1-\alpha)\Phi_{m-1/2,i}; \quad i=1,2,\ldots,I \quad m=1,2,\ldots,M. \qquad (28)$$

($\alpha = 1/2$; diamond & $\alpha = 1$; step scheme).

Equations (27) and (28) add 2IM equations to the IM equations (25), and even using the M boundary conditions, it is still missing I equations to solve the problem. These additional equations are obtained by using the fact that for $\mu = -1 (\mu_{1/2})$, $a_{1/2} = a_{-1/2} = 0$, and therefore equation (25), for this particular direction, is the same as in plane geometry, and the angular fluxes $\Phi_{1/2,i+1/2}$ can be computed by the same scheme discussed before. Then, $\Phi_{1/2,i}$, $i = 1/2, 3/2, \ldots, I+1/2$ are known. Now, using equations (27), the fluxes at all mesh points at $m = 1/2$ can be calculated.

To go forward for all other mesh points for $\mu_m < 0$, equations (25), (27) and (28) are combined to yield,

$$\Phi_{m,i} = K^{(1)}_{m,i}\,\Phi_{m,i+1/2} + K^{(2)}_{m,i}\Phi_{m-1/2,i} + K^{(3)}_{m,i}\,Q_{m,i}, \qquad (29)$$

where $K^{(j)}_{m,i}$ are expressed in terms of α; a; A, and B(known).

Then, starting with $\Phi_{1,I+1/2}$ known from the boundary condition, and with $\Phi_{1/2,i}$ known from the previous step, we progress to the left as

$$\Phi_{1,I} = \underset{\text{known}}{K^{(1)}_{1,I}\,\Phi_{1,I+1/2}} + \underset{\text{known}}{K^{(2)}_{1,I}\Phi_{1/2,I}} + \underset{\text{known}}{K^{(3)}_{1,I}\,Q_{1,I}},$$

and the edges fluxes $\Phi_{1,I-1/2}$ and $\Phi_{3/2,I}$ can be computed using equation (27) and (28) as,

$$\Phi_{1,I-1/2} = 2\Phi_{1,I} - \Phi_{1,I+1/2} \quad (\alpha = 1/2),$$

$$\Phi_{3/2,I} = 2\Phi_{1,I} - \Phi_{1/2,I} \quad (\alpha = 1/2).$$

This scheme is repeated for $\Phi_{1,i}$; $i = I-1, I-2, \ldots$ until $X=0$ ($i = 1/2$) is reached, and then start for the next m, $\mu_m < 0$. ($m = 2, \ldots, M/2$).

Once all $\Phi_{m,i}$, $\mu_m < 0$ have been found, the values of the angular fluxes for $\mu_m > 0$ can be found by a similar strategy. In this case eqs. (25); (27) and (28) are combined, to yield,

$$\Phi_{m,i} = K^{(4)}_{m,i}\,\Phi_{m,i-1/2} + K^{(5)}_{m,i}\Phi_{m-1/2,i} + K^{(6)}_{m,i}Q_{m,i}, \qquad (30)$$

and, starting with $\Phi_{M+1/2,1/2}$ known the boundary conditions or reflective conditions, we progress to the right. Figure 3 illustrates this strategy.

The iteration described above ("inner iteration") gives the angular fluxes at all mesh points in the phase- space for a given source (Q). There are several acceleration schemes to increase the convergence, such as "coarse mesh rebalance"; "Chebysheff"; "synthetic method", but the discussion of such schemes is beyond the scope of this text. The code ANISN (*) uses the "space point renormalization scalling" /21/. For convergence criteria, there are two options:

i) integral convergence test,

$$\frac{1}{V}\int \frac{\Phi^{(n)} - \Phi^{(n-1)}}{\Phi^{(n)}}\, dV < \varepsilon, \qquad (31)$$

ii) point wise flux convergence criteria,

$$\max \left[\frac{\Phi^{(n)} - \Phi^{(n-1)}}{\Phi^{(n)}} \right] < \varepsilon \, . \qquad (32)$$

Once the inner iteration convergence is obtained in the first group (g=1), calculation proceeds until converged inner solutions are obtained in each other g=2,3,...IGM. The downscattering portion of the source to each succeeding group is recomputed as soon as flux information is available. If fission or upscattering is present, the iteration must be continued because these sources depend upon the flux being calculated. This cycle is called "outer iteration". (see figure 1). To accelerate convergence in the outer iteration (mainly when upscattering is present), discrete ordinates codes such as ANISN, use an

* - ANISN-PC (CCC-0514/02) used during the workshop, uses for inner-iteration stabilized variable-mesh rebalancing scheme, or linear diffusion synthetic scheme.

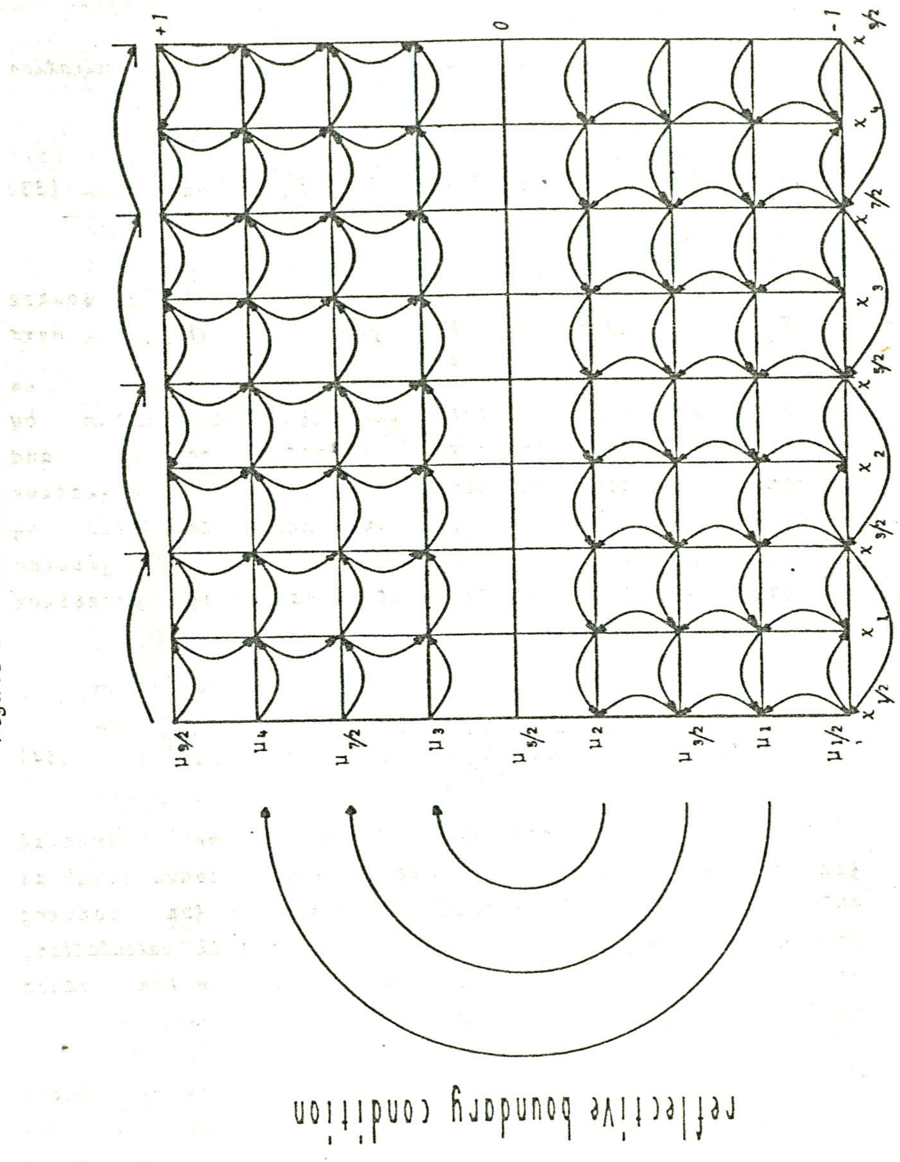


Figure 3 - Discrete Ordinates Strategy Solution

upper scaler factor, which improves eigenvalue convergence and is used to adjust the level of all fluxes before another outeriteration is performed.

After an outer iteration is performed, the multiplication ratio,

$$\lambda = \sum_i V_i (F_i^{(n)} + \sum_g S_{g,i}^{ext}) / \sum_i V_i (F_i^{(n-1)} + \sum_g S_g^{ext}), \qquad (33)$$

is computed, with $S_{g,i}^{ext}$ representing the external source and F_i the fission source $(\Sigma\nu\Sigma f i g \phi_{i,g})$. For the next iteration, a renormalization of the fission source is performed by multiplying the initial fission spectrum by $1/\lambda$, so that λ tends to unity as iteration proceeds, and convergence is achieved when $/1-\lambda/< \varepsilon$. The effective multiplication factor, K_{eff}, is obtained as the ratio of the initial fission spectrum to the current fission spectrum sum. It is also the multiplication of sucessive multiplication ratios, or,

$$K = \sum_g X_g^{initial} \; / \; \sum_g X_g^{current} , \qquad (34)$$

Finally it is interesting to mention some special features of the discrete ordinate transport codes (such as ANISN) that allows these codes to be applied for solving problems in multiplying media; shielding; cell calculation, as well as to be used as auxiliary calculation for other methods, such as Monte Carlo:

i) The outer iteration allows the solution of fixed source, or multiplying media, or combination of these two. This allows several types of applications: K - calculation; α - calculation (time absorption calculation); concentration search calculation (mixture, or element in mixture); zone thickness search calculation and outer radius dimension to achieve a desired multiplication level. In criticality search, the desired parameter is altered to make λ appoach unity.

ii) Besides the solution of forward transport equation, ANISN can perform Adjoint calculation. The adjoint flux, $\Phi^+(\underline{r},\underline{\Omega},E)$ is interpreted as the "importance" of a particle in contributing to detector response at a certain point in phase-space, and it is the solution of the Adjoint transport equation:

$$-\underline{\Omega}.\nabla\Phi^+ + \Sigma\Phi^+ = \iint \Sigma(\underline{r},\underline{\Omega},E\to\underline{\Omega}',E')\,\Phi^+(\underline{r},\underline{\Omega}',E')\,d\underline{\Omega}'dE' + RD, \qquad (35)$$

where RD is the detector response function. The adjoint calculation allows the discrete ordinates codes to be used in several applications such as in Monte Carlo codes, such as MORSE, to be used as importance function in variance reduction techniques; in perturbation theory, to calculate reactivity changes or worth due to material perturbations in regions (ex: control rods), i.e.,

$$\frac{\Delta K}{K} - \iiint \Phi^+(\underline{r},\underline{\Omega},E)\,\delta\Sigma\Phi(\underline{r},\underline{\Omega},E)\,d\underline{\Omega}dEdV$$

and also in the calculation of kinetics parameters, such as β_{eff} (delayed neutron fraction) or ℓ^* (prompt neutron life time).

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