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VOLUME 3

SYNTHESIS OF CALCULATIONAL METHODS FOR THE DESIGN AND ANALYSIS OF RADIATION SHIELDS FOR NUCLEAR ROCKET SYSTEMS

TAPAT

THE FORTRAN IV PROGRAM SYSTEM (THE ANALYSIS PROGRAM AND TRANSPORT)

by

R. K. Disney

Contract No. NAS-8-20414
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ABSTRACT

This report is Volume 3 of nine volumes of the final report on "Synthesis of Calculational Methods for the Design and Analysis of Radiation Shields for Nuclear Rocket Systems". Presented in this volume is a description of the TAPAT program system. The TAPAT program system consists of five FORTRAN IV subprograms, which are as follows:

1) The ADDICT diffusion theory program which solves the multigroup diffusion equations in one-dimensional slab, cylindrical, or spherical geometries.

2) The MIST transport theory program which solves the multigroup S_n transport equations in one dimensional slab geometry.

3) The TOPIC transport theory program which solves the multigroup S_n transport equations in one-dimensional cylindrical geometry.

4) The MISPHT transport theory program which solves the multigroup S_n transport in one-dimensional spherical geometry.

5) The FLUX EDIT data processing program which calculates reaction rates, distributed fixed sources, separable spatial and energy source distributions, and other radiation quantities of interest.

The TAPAT subprograms ADDICT, MIST, MISPHT, and TOPIC are modifications of previously coded diffusion and S_n transport programs. The input data and internal operations of each program are standardized in a single program system called TAPAT. The TAPAT program system provides a complete, neutron and photon, one dimensional radiation analysis of a reactor system in a single computer run. This Fortran IV program uses the overlay mode of the IBM 7094 computer IBSYS Version 13 Monitor System.

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SECTION

1.0 INTRODUCTION

This report is Volume 3 of nine volumes of the final report on "Synthesis of Calculational Methods for the Design and Analysis of Radiation Shields for Nuclear Rocket Systems". Presented in this volume is a description of the TAPAT program system. This TAPAT program system is part of the "early" design method provided for the Marshall Space Flight Center (MSFC), as shown schematically in Figure 1 and discussed in detail in Volume 1. The starting point for the method is the POINT program (Volume 2) which prepares cross section and other basic data for use in the TAPAT program.

In the "early" design method (Figure 1), the TAPAT program system (Volume 3) computes one dimensional neutron and photon energy fluxes in the reactor geometry. From these fluxes, neutron and photon multienergy group sources and distributions are obtained and are used as input to the KAP-V program. The KAP-V program (Volume 4) provides gamma ray and fast neutron radiation levels at locations external to the reactor. Radiation levels from the KAP-V program at a specific radial distance from the center of the reactor can then be employed in the TIC-TOC-TOE program (Volume 5) for calculating radiation quantities of interest in an on-axis liquid hydrogen propellant tank.

The TAPAT program system evolved from a series of one-dimensional S_n transport programs written by D. M. Shapiro (formerly of Internuclear Company) and G. E. Putnam (at Phillips Petroleum Company). This series includes three separate programs which use the direct angular flux technique for solving the S_n equations. The three programs were originally FORTRAN II versions in slab (MIST)[1], spherical (MISPHT)[2], and cylindrical (TOPIC)[3] geometry solutions in the S_n approximation to the Boltzmann transport equation. Each geometry required a slightly different numerical solution and the three programs were not compatible as far as input preparation and operation.

In 1964, the input data preparation and program operation of each program was standardized and integrated into a single system package called the WANL TAPAT System. This was achieved by reducing the numerical approximation and problem size capability such

that there are some restrictions on the number of groups, angular approximation, and mesh intervals. These programs were linked in the TAPAT system by a common routine (FLUX EDIT) so that a series of problems can be run as change cases with very few input data changes.

Since 1964, the TAPAT system has been extended to accept cross section data as tape input. The FLUX EDIT routine has been modified so that distributed fixed source problems could either be input with a minimum of preparation or could be calculated from a neutron problem for immediate use in a photon transport problem. This feature allows a single computer problem run for a complete one dimensional neutron and photon radiation analysis. During this period, a diffusion theory program similar to the Atomics International AIM-5[4] or AIM-6 programs was added with input requirements compatible with the other TAPAT programs. Thus, one program (ADDICT) solves all three geometries (slab, sphere, or cylinder) in the diffusion approximation.

Finally, the capability of group upscatter was incorporated into the TAPAT programs for analyses of graphite moderated nuclear rocket reactors.

During this contract period (Contract NAS-8-20414), the FORTRAN IV version of the TAPAT system using the overlay mode of IBM-7094 IBSYS, Version 13 Monitor System was made operational on the MSFC computer. This FORTRAN IV version of the TAPAT system, which is compatible with an IBM-7094 computer with 32K memory, has the following capabilities:

1) Maximum number of energy groups - 20
2) Maximum number of regions - 30
3) Maximum number of materials - 30
4) Maximum number of downscatter groups - up to and including 6 groups
5) Maximum number of upscatter groups - up to and including 5 groups
6) Maximum angular quadrature (S_n order) - 4

Section 2 describes various features of the TAPAT program system in sufficient detail to permit an understanding of the diffusion, transport, and FLUX EDIT subprograms. Further details on the basic diffusion and transport routines are available in the original references.

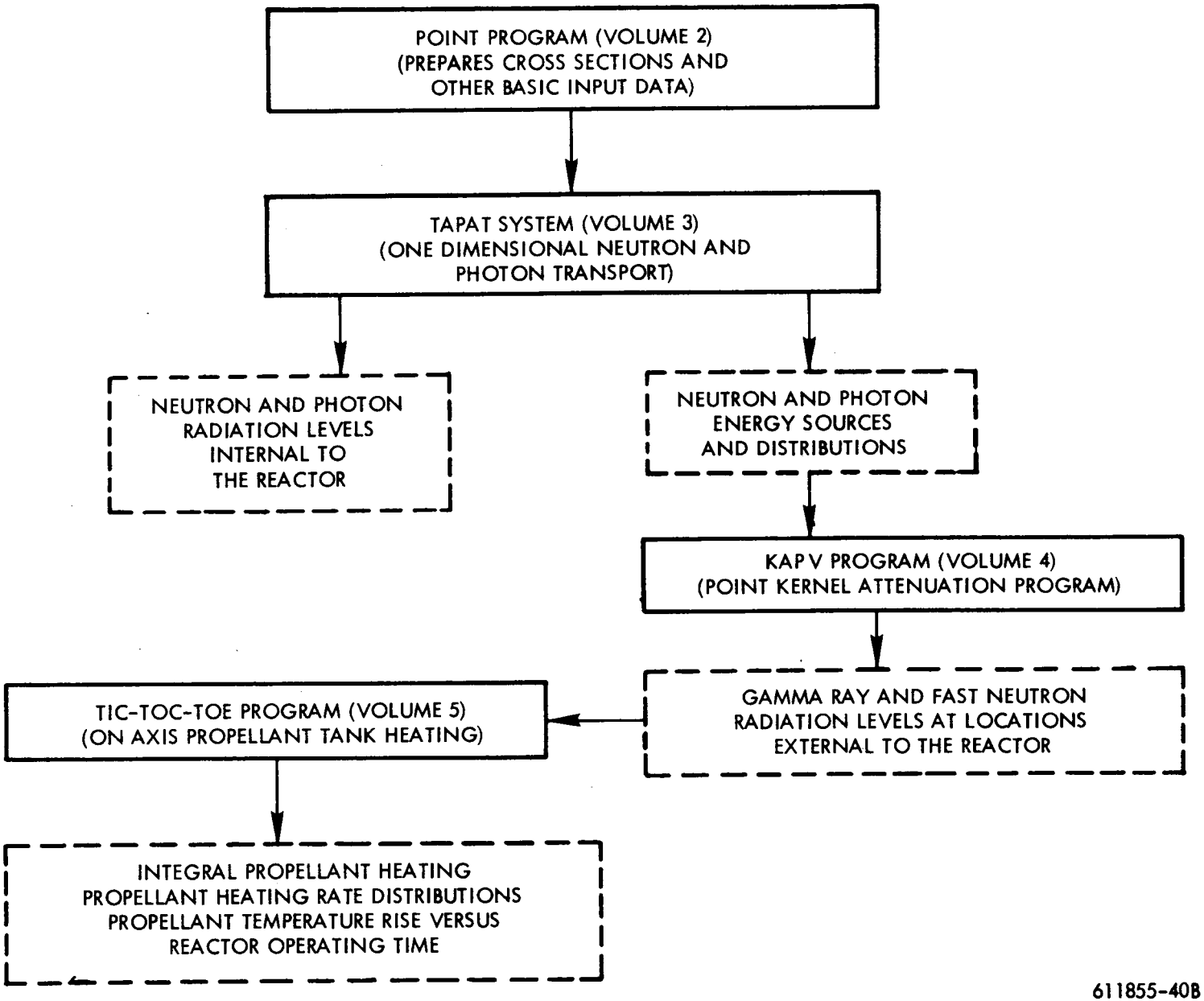


Figure 1. Schematic Diagram of the "Early" Design Method

A description of input data requirements is given in Section 3. The structure of the TAPAT system is given in Section 4. Because the TAPAT, FORTRAN IV source program contains approximately 12,000 FORTRAN statement cards, no listing of the source program is included in this report. This listing is available on request from the authors or Mr. H. E. Stern of Marshall Space Flight Center.

SECTION

2.0 GENERAL DESCRIPTION OF THE PROGRAMS

The TAPAT program system consists of five FORTRAN IV subprograms that (1) solve the one-dimensional Boltzmann transport equation using S_n transport and/or diffusion approximations, and (2) perform data processing functions to provide a complete (neutron and photon) radiation analysis of a nuclear reactor or radiation source. These five subprograms are:

1) The ADDICT diffusion theory program which solves the multigroup diffusion equations in one-dimensional slab, cylindrical, or spherical geometries.

2) The MIST transport theory program which solves the multigroup S_n transport equations in one-dimensional slab geometry.

3) The MISPHT transport theory program which solves the multigroup S_n transport equations in one-dimensional spherical geometry.

4) The TOPIC transport theory program which solves the multigroup S_n transport equations in one-dimensional cylindrical geometry.

5) The FLUX EDIT data processing program which calculates reaction rates, distributed neutron and photon fixed sources, separable spatial neutron and photon energy source distributions, and other radiation quantities of interest, such as heating rates.

There are five types of problems which can be solved with the TAPAT program. These are:

Type 1: An eigenvalue problem with no fixed (distributed or boundary) sources.

Type 2: A fixed (distributed or boundary) source problem with no fissions.

Type 3: A fixed (distributed or boundary) source problem with fissions.

Type 4: A concentration search problem where a specified concentration is varied until a desired eigenvalue is reached.

Type 5: A region thickness search problem where a specified region thickness is varied until a desired eigenvalue is reached.

The TAPAT subprograms are modifications of original diffusion and S_n transport programs (ADDICT, MIST, MISPHT, and TOPIC). The following subsections are subdivided into discussions of:

1) The diffusion equations and boundary conditions of the ADDICT program.

2) The S_n transport equations, boundary conditions, and the numerical approximations used in their solutions.

3) A discussion of the

a) energy coupling multigroup equation (diffusion or S_n transport approximation) solution in TAPAT, and

b) outer iteration cycle in TAPAT.

4) The FLUX EDIT subprogram and its numerical operations.

A schematic diagram of the TAPAT system is shown in Figure 2. As shown in the figure, the POINT program (Volume 2) prepares the macroscopic neutron and photon cross sections for the neutron and photon transport codes, and the microscopic cross section data for the FLUX EDIT program. The flow of data is, as indicated in figure 2, from the transport code, to FLUX EDIT, to the photon transport code, and again to FLUX EDIT. The TAPAT program can be run as a set of stacked problems to provide a complete one-dimensional analysis in one run on the computer.

2.1 DIFFUSION THEORY PROGRAM: ADDICT

The numerical solution in the diffusion theory program, ADDICT, is taken largely from Reference 1 and is identical to the AIM series of programs. The ADDICT program was tailored into the TAPAT system. The following description is intended to acquaint the user of the ADDICT program with its solution; it provides insight into the proper use of ADDICT (e.g., choice of diffusion coefficient, boundary conditions, buckling, etc.) in the TAPAT system.

The diffusion equation for energy group, g, in the multigroup treatment is as follows:

$$- Dg(\vec{r})\,\nabla^2(\vec{r})\,Ng(\vec{r}) + \Sigma_g^t(\vec{r})\,Ng(\vec{r}) = q_g(\vec{r}) \qquad (2.1)$$

where:

$Ng(\vec{r})$ is the neutron flux in group g.

$\nabla^2(\vec{r})$ is the Laplacian flux operator

$Dg(\vec{r})$ is the diffusion coefficient of neutrons in group g

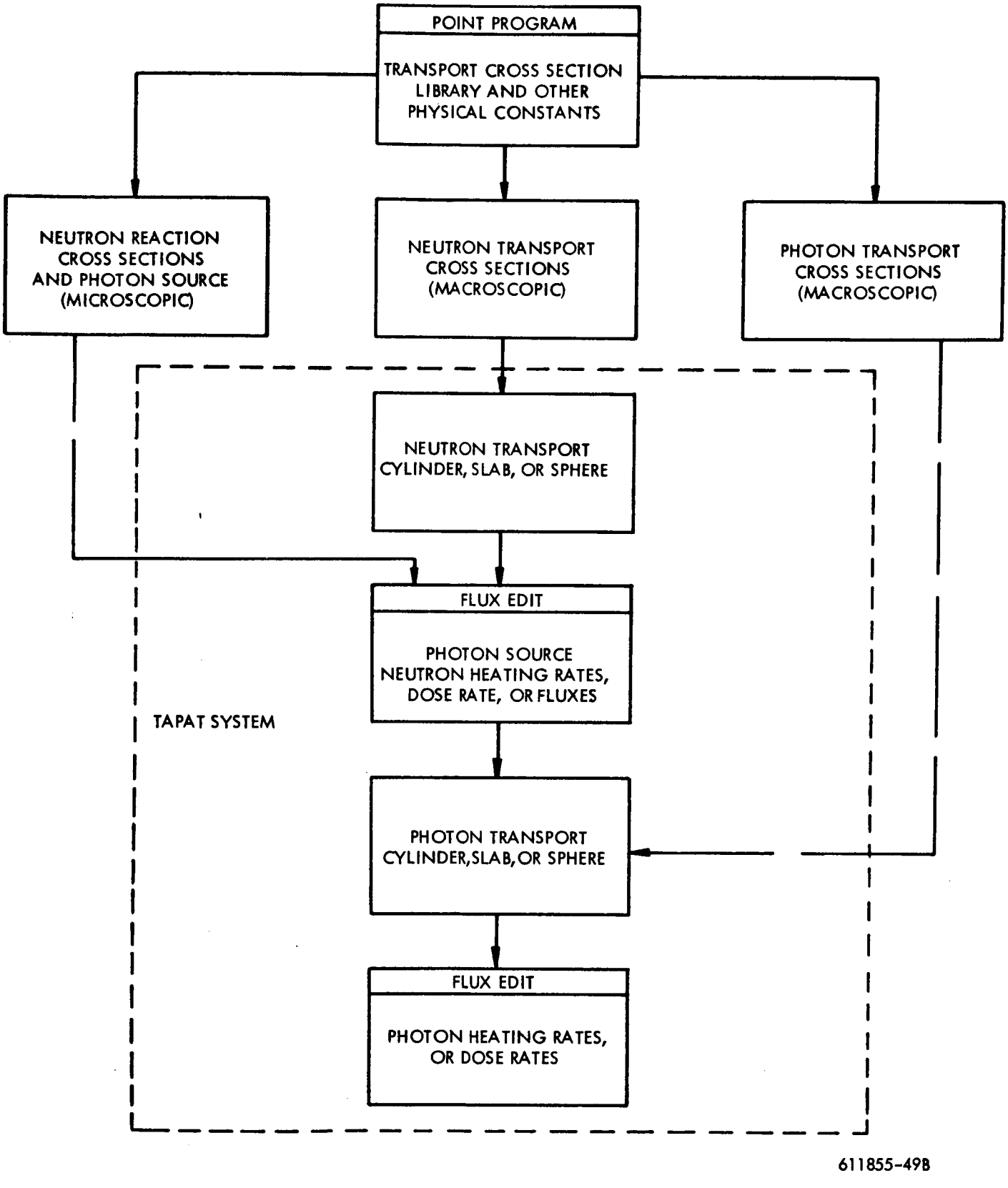


Figure 2. Schematic Diagram of the One Dimensional Transport System (TAPAT)

$\Sigma^t_g(\vec{r})$ is the total removal cross section for neutrons in group g

$q_g(\vec{r})$ is the total fixed source of neutrons in group g which is the summation of three terms. These are:

(1) the fixed volume source of neutrons in group g, $Qg(\vec{r})$.

(2) the fission source of neutrons in group g, $Fg(\vec{r})$

(3) the scattering source of neutrons into group g from group g'.

Solution of this diffusion equation as described in Reference 1 is accomplished by using central difference methods to approximate the derivatives at each mesh point in slab, cylindrical, or spherical geometry problems. The ADDICT program requires that: (1) the material properties be specified in regions, and (2) each region has a constant mesh interval size. The application of flux continuity conditions at each interior region boundary and of surface source leakage boundary conditions at the external boundaries results in a system of linear equations which can be solved by recursion relations.

The groupwise cross sections used in ADDICT are developed from the transport cross section sets normally used in the transport theory subprograms of TAPAT. These quantities are described in the following sections.

2.1.1 Total Removal Coefficient

The total removal coefficient $\Sigma^t_g(\vec{r})$ used in ADDICT is defined as the sum of the transverse leakage coefficient ($DgBg^2$) and the removal cross section, $\Sigma^R_g(\vec{r})$. The group removal cross section is defined as:

$$\Sigma^R_g(\vec{r}) = \Sigma^t_g(\vec{r}) - \Sigma^{S_0}_{g \rightarrow g}(\vec{r})$$

where:

$\Sigma^t_g(\vec{r})$ = the total (or transport corrected) cross section for group, g, at $\vec{r}$

$\Sigma^{S_0}_{g \to g}(\vec{r})$ = the within group isotropic (i.e. zeroth moment) scattering cross section (or transport corrected form of this quantity) for group, g, at $\vec{r}$.

It can be seen that ADDICT assumes that $\Sigma^{R}_{g}(\vec{r})$ is independent of the transport correction made to $\Sigma^{S_0}_{g \to g}(\vec{r})$ and $\Sigma^{t}_{g}(\vec{r})$.

2.1.2 Diffusion Coefficients

The ADDICT program has two options for developing the diffusion coefficients for each group. Diffusion coefficients for each group and region mixture may be input to the program, or the program will calculate mixture diffusion coefficients. The calculation of the diffusion coefficient, Dg $(\vec{r})$, is performed for region materials only, and the region material cross sections must be a set of data calculated internally to the program (i.e., the region material number MIR for region, m, must appear in the mixture vector, MIX, as a mixture of one or more sets of cross section data). The options for calculating Dg $(\vec{r})$ are:

$$Dg(\vec{r}) = \frac{1}{3\,\Sigma^{t}_{g}(\vec{r})} \quad \text{or} \quad \frac{1}{3\,\Sigma^{t}_{g}(\vec{r})\;\kappa^{2}},$$

$$\kappa^{2} = \left[1 - \frac{4\,\Sigma^{a}_{g}(\vec{r})}{5\,\Sigma^{t}_{g}(\vec{r})}\right]^{2}$$

where:

$\Sigma^{t}_{g}(\vec{r})$ = the total (i.e., transport corrected) cross section for group g at $\vec{r}$.

$\Sigma^{a}_{g}(\vec{r})$ = the absorption cross section for group g at $\vec{r}$, defined as:

$$\Sigma^{a}_{g}(\vec{r}) = \Sigma^{t}_{g}(\vec{r}) - \sum_{g' \neq g} \Sigma^{S_0}_{g' \to g}(\vec{r})$$

$\Sigma^{S_0}_{g' \to g}$ = the isotropic scattering cross section for scatter-transfer from group g' to g at $\vec{r}$.

The user specifies which option is used by the input quantity MUTEST. The second equation for Dg and κ^2 is defined in Reference 5.

2.1.3 Fixed Source

Total fixed source $q_g(\vec{r})$ in each group, g at $\vec{r}$, is the summation of three terms. These terms are:

1) the fixed volume source of neutrons $Qg(\vec{r})$ per unit volume per second.

2) the fission source of neutrons, $Fg(\vec{r})$, which is equal to the number of neutrons per unit volume per second. This quantity is defined as:

$$Fg(\vec{r}) = \frac{\chi_g}{\lambda} \sum_{g'=1}^{G} \nu_{g'} \Sigma^f_{g'}(\vec{r}) N_{g'}(\vec{r})$$

where

λ = 1.0 in distributed or boundary fixed source problems. In eigenvalue problems, λ = the eigenvalue obtained in the previous outer iteration.

χ_g = the fraction of total neutrons released in a fission event which appear in group g.

$\nu_{g'} \Sigma^f_{g'}(\vec{r})$ = the neutron fission production cross section which is the product of neutrons produced per fission ($\nu g'$) times the fission cross section $\left(\Sigma^f_{g'}\right)$ for the g' group.

$N_{g'}(\vec{r})$ = the neutron flux in group g' which is the multigroup flux data from the previous outer iteration

3) the scattering source of neutrons in group g. This term is the number of neutrons per unit volume scattered from group g' into group g. The neutron flux data $Ng'(\vec{r})$ is obtained from the outer iteration multigroup fluxes for higher energy groups which scatter into the lower energy group g (i.e., downscatter) and from previous outer iteration multigroup fluxes for lower energy groups which scatter into the higher energy group (i.e., upscatter).

2.1.4 Boundary Conditions

At the left and right boundaries of a problem (i = 1 and i = MAX) there are four boundary condition options available in the ADDICT program. These options are identical to the AIM program series[1-4] options. The boundary conditions are specified by the input values, $ALPHA_{bg}$ for boundary b (left or right) and group g as:

1) $N_{bg} + \beta_{bg}\left[\frac{dN_{bg}}{dr}\right]_b = 0.0$ $\qquad (ALPHA_{bg} = 0.0)$

2) $\left[\frac{dN_{bg}}{dr}\right]_b = 0.0$ $\qquad (ALPHA_{bg} = 1.0)$

3) $N_{bg} = 0.0$ $\qquad (ALPHA_{bg} = 2.0)$

4) $N_{bg} = \Delta bg$ $\qquad (ALPHA_{bg} = 3.0)$

The quantity β_{bg} is defined as the group dependent extrapolation length at either boundary, and N_{bg} is the flux at the boundary b, for group, g. A discussion of the derivation of these quantities is given in Appendix 4 of Reference 1. The final equations of β_{bg} for the inner and outer (left and right) boundaries are presented here.

At the (left and right) boundaries of a problem β_{bg} is defined as:

$$\beta_{bg}\,(LEFT) = \frac{3.0*Dg*\ 0.710446 + (1.080417*\xi g)}{1.0 + (0.8103127*\xi g)}$$

$$\beta_{bg}\,(RIGHT) = \frac{3.0*Dg*0.710446}{1.0 + (0.710446*\xi g)}$$

where:

β_{bg} = the group dependent extrapolation length,

$\xi_g = \frac{3.0*P*Dg}{2.0*R}$

R = the radius (or mesh point dimension) at the left or right boundary.

P = the geometry parameter in the above equation, and,

P = 0.0 for slab geometry

P = 1.0 for cylindrical geometry

P = 2.0 for spherical geometry

Dg = the group diffusion coefficient of the material in the region at the left or right boundary.

The user has the option of providing group dependent β_{bg}'s as input data or using the above equations for obtaining the group dependent β_{bg}'s.

2.2 TRANSPORT THEORY PROGRAMS: MIST, MISPHT, TOPIC

The major portion of the following discussion is taken from References 6, 7, and 8 to illustrate the numerical solution in the transport theory programs, MIST, MISPHT, and TOPIC. The original work performed on the S_n transport methods by G. E. Putnam and D. M. Shapiro was incorporated into a consistent package at WANL with the assistance of D. M. Shapiro as consultant. The linkage of these three programs in a system with consistent input data and numerical solution capability (e.g., number of groups, number of mesh points, etc.) comprise the bulk of the work performed at WANL on the TAPAT system.

2.2.1 Boltzmann Transport Equation

The Boltzmann transport equation for the time and energy independent case is:

$$\text{div}\ \vec{N}(\vec{r},\vec{\Omega}) + \Sigma^t(\vec{r},\vec{\Omega})\, N(\vec{r},\vec{\Omega}) = \int_{\vec{\Omega}'} \Sigma^s(\vec{r},\vec{\Omega},\vec{\Omega}')\, N(\vec{r},\vec{\Omega}')\, d\Omega' + q(\vec{r},\vec{\Omega}) \qquad (2.2)$$

where:

$\vec{N}(\vec{r},\vec{\Omega})$ = the vector flux defined as the number of neutrons or photons traveling in the direction $\vec{\Omega}$ crossing a unit area normal to $\vec{\Omega}$ per unit time.

$\Sigma^t(\vec{r},\vec{\Omega})$ = the total cross section for removal of neutrons or photons from $d\vec{\Omega}$ about $\vec{\Omega}$.

$\Sigma^s(\vec{r},\vec{\Omega},\vec{\Omega}')$ = the total scattering cross section for scattering of neutrons or photons in $d\vec{\Omega}'$ about $\vec{\Omega}'$ into $d\vec{\Omega}$ about $\vec{\Omega}$.

$q(\vec{r},\vec{\Omega})$ = the total source of neutrons or photon energy per unit volume per unit solid angle per unit time emitted in $d\vec{r}$ about $\vec{r}$ and $d\vec{\Omega}$ about $\vec{\Omega}$.

2.2.2 Slab Geometry: MIST

Consider equation 2.2 in slab geometry in which the flux and source are functions only of the space variable, x, and some angle θ, between a unit vector in the positive, x, direction and $\vec{\Omega}$. Further, let $\cos\theta = \mu$. Then $N(\vec{r},\vec{\Omega}) = N(x,\mu)$ and $q(\vec{r},\vec{\Omega}) = q(x,\mu)$. Then the first term in equation 2.2 can be reduced by the well-known identity:

$$\begin{aligned}\text{div}\left[N(\vec{r},\vec{\Omega})\vec{\Omega}\right] &= \text{grad } N(x,\vec{\Omega})\cdot\vec{\Omega} + N(x,\vec{\Omega})\,\text{div}\,\vec{\Omega}\\ &= \text{grad } N(x,\vec{\Omega})\cdot\vec{\Omega}\\ &= \vec{\Omega}\cdot\vec{x}\,\frac{\partial N(x,\vec{\Omega})}{\partial x}\\ &= \mu\,\frac{\partial N(x,\vec{\Omega})}{\partial x}\end{aligned}$$

($\vec{x}$ is the unit vector in the x direction.)

Setting $d\Omega = d\phi d\mu$ in equation 2.2 leads to the result:

$$\mu\frac{\partial N(x,\mu)}{\partial x} + \Sigma^t(x)\,N(x,\mu) = \int_0^{2\pi}\int_{-1}^{1}\Sigma^s(x,\vec{\Omega},\vec{\Omega}')\,N(x,\mu')\,d\mu'\,d\phi' + q(x,\mu) \qquad (2.3)$$

where the substitution $f(x,\mu) = f(\vec{r},\vec{\Omega})$ has been made.

Now, it is assumed that the scattering cross section is a function only of the angle θ_o between $\vec{\Omega}$ and $\vec{\Omega}'$, so that if $\mu_o = \cos\theta_o$, then

$$\Sigma^s(x,\mu_o) = \Sigma^s(x,\vec{\Omega},\vec{\Omega}')$$

The representation of $\Sigma^s(x, \mu_o)$ in a spherical harmonics expansion is given as

$$\Sigma^s(x,\mu_o) = \sum_{l=0}^{\infty} \Sigma^s_l(x) P_l(\mu_o) \left[\frac{2l+1}{4\pi}\right] \tag{2.4}$$

where

$$\Sigma^s_l(x) = \int_0^{2\pi} \int_{-1}^{1} \Sigma^s(x, \mu_o) P_l(\mu_o) d\mu_o d\phi;$$

and, if one uses the addition theorem for spherical harmonics,

$$P_l(\mu_o) = P_l(\mu) P_l(\mu') + 2 \sum_{m=1}^{l} \left[\frac{(l-m)'}{(l+m)'}\right] P_l^m(\mu) \quad P_l^m(\mu') \cos m(\phi-\phi') \tag{2.5}$$

(where the P_l^m's are the associated legendre polynomials).

These relationships can be used to reduce the basic Boltzmann equation in slab geometry to:

$$\mu \frac{\partial N(x,\mu)}{\partial x} + \Sigma^t(x) N(x,\mu) = \sum_{l=0}^{\infty} \left[\frac{2l+1}{2}\right] \Sigma^s{}'_l(x) P_l(\mu) \int_{-1}^{1} P_l(\mu') N(x,\mu') d\mu' + q(x,\mu) \tag{2.6}$$

The terms involving m, in equation 2.5, vanish with integration over ϕ'. Equation 2.6 is the basic equation used for each energy group in the MIST program.

2.2.3 Spherical Geometry: MISPHT

Consider equation 2.2 in spherical geometry where the flux and source are functions only of a radial coordinate, r, and some angle, θ, between a unit vector in the positive r direction and $\vec{\Omega}$. In this case, $N(x,\mu)$ in the previous treatment is replaced by $N(\vec{r},\vec{\Omega})$, and $q(r,\mu)$ replaces $q(\vec{r},\vec{\Omega})$ where $\mu = \cos\theta = [\vec{r}\cdot\vec{\Omega}]/r$. The first term in equation 2.2 can be reduced by a well-known identity:

$$\begin{aligned}\text{div}\,[N(\vec{r},\vec{\Omega})\vec{\Omega}] &= \text{grad}\,N(r,\vec{\Omega})\cdot\vec{\Omega} + N(r,\vec{\Omega})\,\text{div}\,\vec{\Omega} \\ &= \text{grad}\,N(r,\vec{\Omega})\cdot\vec{\Omega} \\ &= \vec{\Omega}\cdot\vec{i}_r\frac{\partial N(r,\mu)}{\partial r} + \frac{\partial N(r,\mu)}{\partial \mu}\left[\vec{\Omega}\cdot\text{grad}\left(\frac{\vec{r}\cdot\vec{\Omega}}{r}\right)\right]\end{aligned}$$

Now: $\vec{\Omega}\cdot\text{grad}\left(\dfrac{\vec{r}\cdot\vec{\Omega}}{r}\right) = \dfrac{\vec{\Omega}\cdot\vec{\Omega}}{r} - (\vec{r}\cdot\vec{\Omega})\left[\vec{\Omega}\cdot\text{grad}\,r\right]/r^2,$

and since $\text{grad}\,r = \vec{i}_r$, $\vec{\Omega}\cdot\vec{\Omega} = 1.0$.

Then, $\text{div}\,N(r,\vec{\Omega})\cdot\vec{\Omega} = \mu\dfrac{\partial N(r,\mu)}{\partial r} + \dfrac{(1-\mu^2)}{r}\dfrac{\partial N(r,\mu)}{\partial \mu}$

($\vec{i}_r$ is the unit vector in the r direction and $r\vec{i}_r = \vec{r}$.) Setting $d\Omega = d\phi d\mu$ in equation 2.2 leads to the result:

$$\mu\frac{\partial N(r,\mu)}{\partial r} + \frac{1-\mu^2}{r}\frac{\partial N(r,\mu)}{\partial \mu} + \Sigma^t(r)\,N(r,\mu)$$

$$= \int_0^{2\pi}\int_{-1}^{1} \Sigma^s(r,\vec{\Omega},\vec{\Omega}')\,N(r,\mu')\,d\mu' d\phi' + q(r,\mu) \qquad (2.7)$$

If the relationships of the scattering cross sections as shown above in the slab geometry solution are used in equation 2.7, the basic Boltzmann transport equation in spherical geometry reduces to:

$$\mu \frac{\partial N(r,\mu)}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial N(r,\mu)}{\partial \mu} + \Sigma^t(r)\, N(r,\mu)$$

$$= \sum_{l=0}^{\infty} \frac{2l+1}{2} \Sigma^{sl}(r) P_l(\mu) \int_{-1}^{1} P_l(\mu') N(r,\mu')\, d\mu' \qquad (2.8)$$

Equation 2.8 is the basic equation used for each energy group in the MISPHT program.

2.2.4 Cylindrical Geometry: TOPIC

Consider equation 2.2 in cylindrical geometry where the flux and source are functions of the space variable, r, and the angles, θ and ϕ, between a unit vector in the positive r direction and $\vec{\Omega}$. In this case $N(\vec{r},\vec{\Omega}) = N(r,\mu,\phi)$, and $q(\vec{r},\vec{\Omega}) = q(r,\mu,\phi)$, where $\vec{\Omega}$ is the unit vector in the direction μ, ϕ, and where $\mu = \cos\theta$.

It is assumed in TOPIC that there is no variation of the angular distribution of the flux in either the Z direction (parallel to the cylinder axis) and that there is azimuthal symmetry about the centerline of the problem (i.e. in the ϕ direction of figure 3), but not about the solution point (in the ϕ direction). The derivation of the Boltzmann transport equation in cylindrical coordinates is presented in References 8 and 9 and the equation solved in each energy group is given as follows:

$$\frac{\sqrt{1.0-\mu^2}\cos\phi}{r} \frac{\partial[r\, N(r,\mu,\phi)]}{r} - \frac{\sqrt{1.0-\mu^2}}{r} \frac{\partial\{[\sin\phi][N(r,\mu,\phi)]\}}{\partial\phi}$$

$$+ \Sigma^t(r)\, N(r,\mu,\phi) = \int_0^{2\pi} \int_{-1}^{1} \Sigma^s(r,\mu_o)\, N(r,\mu',\phi')\, d\mu' d\phi' + q(r,\mu,\phi) \qquad (2.9)$$

Figure 3 illustrates the cylindrical coordinate system where the unit vector $\vec{\Omega}$ in the direction μ,ϕ is shown. The angle, θ, is the polar angle between the Z direction and $\vec{\Omega}$, and ϕ is the azimuthal angle between the plane defined by the radial (r) and axial (Z) coordinate axes and the rotated plane defined by the r' and Z coordinate axes.

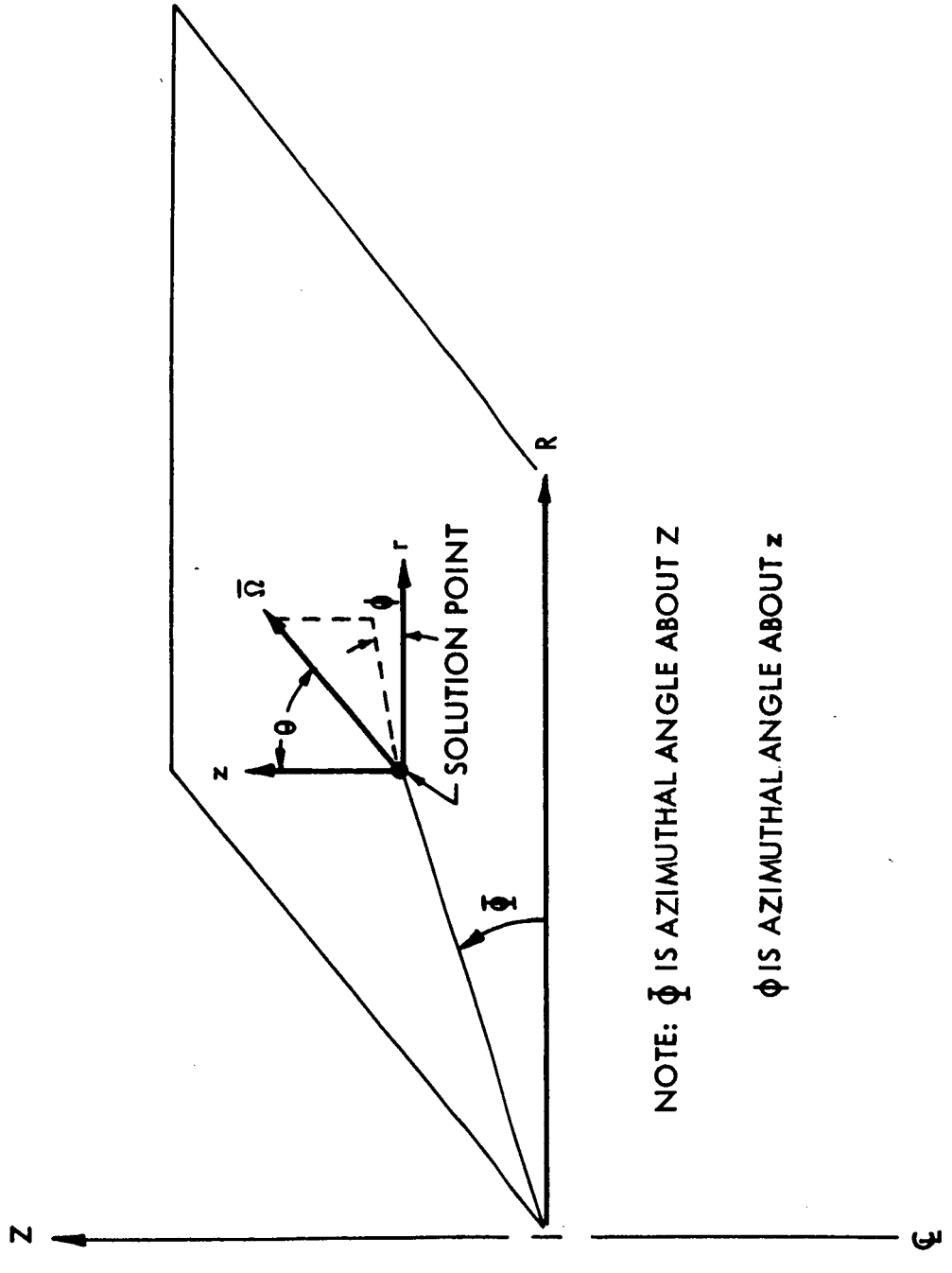


Figure 3. Cylindrical Coordinate System

The integration of the scattering integral:

$$S(r,\mu',\phi') = \int_0^{2\pi} \int_{-1}^{1} \Sigma^s(r,\mu_o)\, N(r,\mu'\phi')\, d\mu' d\phi'$$

of equation 2.9 and of the $q(r,\mu,\phi)$ term becomes complex in cylindrical coordinates because of the inclusion of angle Φ. The derivation and numerical solution of these quantities are presented in Reference 8.

2.2.5 Numerical Approximations

The numerical approximations in the solution of the group difference equations for the TAPAT transport theory subprograms are summarized as follows:

1) In each of the three subprograms:

a) the scattering functions, $\Sigma^s(x,\mu_o)$ or $\Sigma^s(r,\mu_o)$, are represented by a Legendre series.

b) the cross sections are constant with respect to x or r in a region and all mesh intervals on x or r (i.e., Δx or Δr) are the same within each region.

c) the integral for the scattering within a group is limited to an $l = 1$ (i.e., P_1 only) scattering cross section approximation and all other scattering (down scatter or upscatter) is assumed isotropic.

2) In the MIST and MISPHT subprograms the flux $N_g(x,\mu)$ or $N_g(r,\mu)$ is assumed to be linear with respect to x or r and μ ($\mu = \cos\theta$) in each interval. This approximation leads to the expression in either x or r that in the x interval (x_i, x_{i+1}) and the μ interval (μ_j, μ_{j+1}) the flux $N(x,\mu)$ follows

$$N(x,\mu) = N(x_i,\mu_j) + \frac{\partial N(x_i,\mu_j)}{\partial x}(x - x_i) + \frac{\partial N(x_i,\mu_j)}{\partial \mu}(\mu - \mu_j) + \frac{\partial^2 N(x_i,\mu_j)}{\partial x\, \partial \mu}(x - x_i)(\mu - \mu_j)$$

where:

$$\frac{\partial N(x_i,\mu_j)}{\partial x} = \frac{N(x_{i+1},\mu_j) - N(x_i,\mu_j)}{x_{i+1} - x_i}$$

$$\frac{\partial N(x_i,\mu_j)}{\partial \mu} \qquad \frac{N(x_i,\mu_{j+1}) - N(x_i,\mu_j)}{\mu_{j+1} - \mu_j}$$

$$\frac{\partial N(x_i,\mu_j)}{\partial x\,\partial \mu} \qquad \frac{N(x_{i+1},\mu_{j+1}) - N(x_{i+1},\mu_j) - N(x_i,\mu_{j+1}) + N(x_i,\mu_j)}{(x_{i+1} - x_i)\ (\mu_{j+1} - \mu_j)}$$

These equations lead to the division of μ into discrete intervals in the slab or spherical geometries. There are n/2 (n is the S_n or quadrature order) intervals in each half of the μ interval as shown in Figure 4 for S_4 angular segmentation. There are (n/2) + 1 values of the flux $N(x,\mu_j)$ in each half space of μ. In the slab geometry solution, there are two values of the flux $N(x,\mu_j)$ at $\mu_j = 0.0$ (i.e., $\theta = 90$ degrees), to allow for the possible discontinuity of the function $N(x,\mu_j)$ at this point. The solution in the slab or spherical geometries employs symmetry in one variable to reduce the numerical approximation to a simpler form (i.e., $N(x,\mu)$ or $N(r,\mu)$.

3) In the TOPIC subprogram, the flux $N(r,\mu,\phi)$ is assumed to be linear with respect to r and $\cos\phi$ in a manner similar to the MIST and MISPHT subprograms. Since no symmetry exists in the second angle, θ, the TOPIC program uses a Gauss quadrature in the μ half space ($\mu = \cos\theta$) as indicated in Figure 4. The difference equations derived in the variables r and $\cos\phi$ are used in conjunction with the Gauss quadrature points and weights to establish a set of linear equations at each Gauss quadrature point in the variable μ. The complex equation set is fully developed in Reference 8 and the reader is referred to that document for further information.

The equations for cylindrical geometry lead to a division of each $\cos\phi$ halfspace ($\phi = 0$ to $\frac{\pi}{2}$; $\phi = \frac{\pi}{2}$ to π) into n/2 intervals with a total of N intervals in the $\cos\phi$ halfspace. This partitioning is carried through each Gauss quadrature point in the variable μ. Since the μ variable is symmetric about the r-z plane in Figure 3, the partioning of the μ halfspace is limited to the positive μ direction in the interval $\mu = 0.0$ to $\mu = 1.0$. The solution in the μ halfspace used in TOPIC is a unique numerical technique which eliminates the

direct iterative solution of the Gauss point fluxes. As described by Putnam[8], the solution of the difference equations at each Gauss point is iterative in the sense that if there is no anistropic scattering, only one iteration (a single pass) through the Gauss point flux solution is required. If anistropic scattering is included (i.e., $\Sigma^{S}_{g \rightarrow g} l \neq 0.0$), then, because of the numerical techniques used, only a few (i.e., usually less than 3 or 4) inner iterations are required on the Gauss quadrature points to converge the angular fluxes.

4) In each of the subprograms, MIST, MISPHT, TOPIC, the range of the variable r or x is subdivided into I - 1 mesh intervals. Since each region, m, is subdivided into i_m equal size mesh intervals and there are NREG regions, there exists $I = 1 + \sum_{m=1}^{NREG} i_m$ flux solution mesh points.

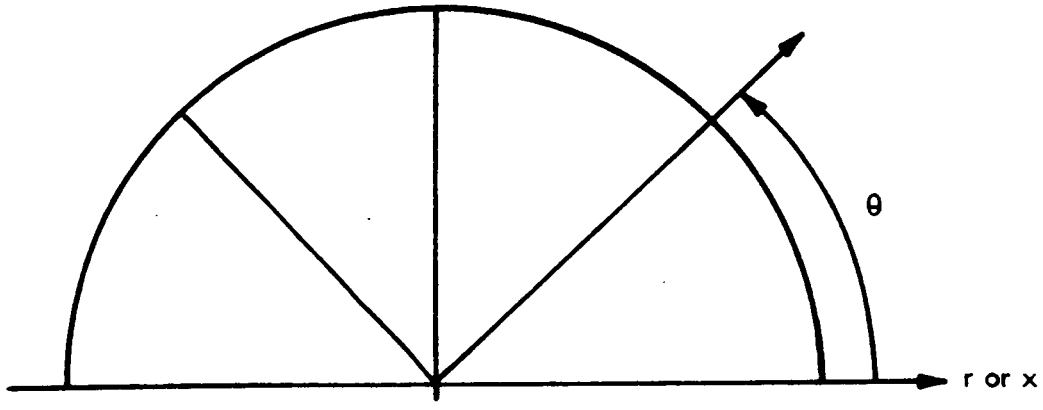
2.2.6 Boundary Conditions

The boundary condition for each group at either boundary is expressed in MIST or MISPHT subprograms by the following equation:

$$N_g(x_b, \mu) = a_{bg} N_g(x_b, -\mu) + 2\beta_{bg} \left| \int_{\Delta\mu_b} N_g(x_b, \mu')\, \mu'\, d\mu' \right| + \sum_{l=0}^{I} \gamma_{lbg}\, P_l(\mu) + \Delta_{bg}(x_b, \mu) \tag{2.10}$$

In this equation, b = boundary (left or right), μ = the cosine of an angle in the angular halfspace which is directed into the boundary surface. Therefore, for the left boundary, $0 \geq \mu \geq 1$; and for right boundary, $-1 \leq \mu \leq 0$. Then, $\Delta\mu$ is the μ halfspace for fluxes emerging from the boundary surface. The physical meaning of each of the terms on the right hand side of equation 2.10 is as follows:

a) If a_{bg} is some number in the interval (0, 1), then the fraction a_{bg} of any flux emerging from the boundary surface will be reflected back into the surface as if reflected by a perfect mirror. This a_{bg} term in the equation is, for example, used in specifying a perfect symmetry condition at a boundary by setting $a_{bg} = 1.0$. The number a_{bg} is termed the mirror albedo coefficient.



TOPIC ANGULAR SEGMENTATION

S_4 ANGULAR QUADRATURE IN COS ϕ AND SECOND ORDER (MIK = 2) ANGULAR QUADRATURE IN μ (μ = COS θ)

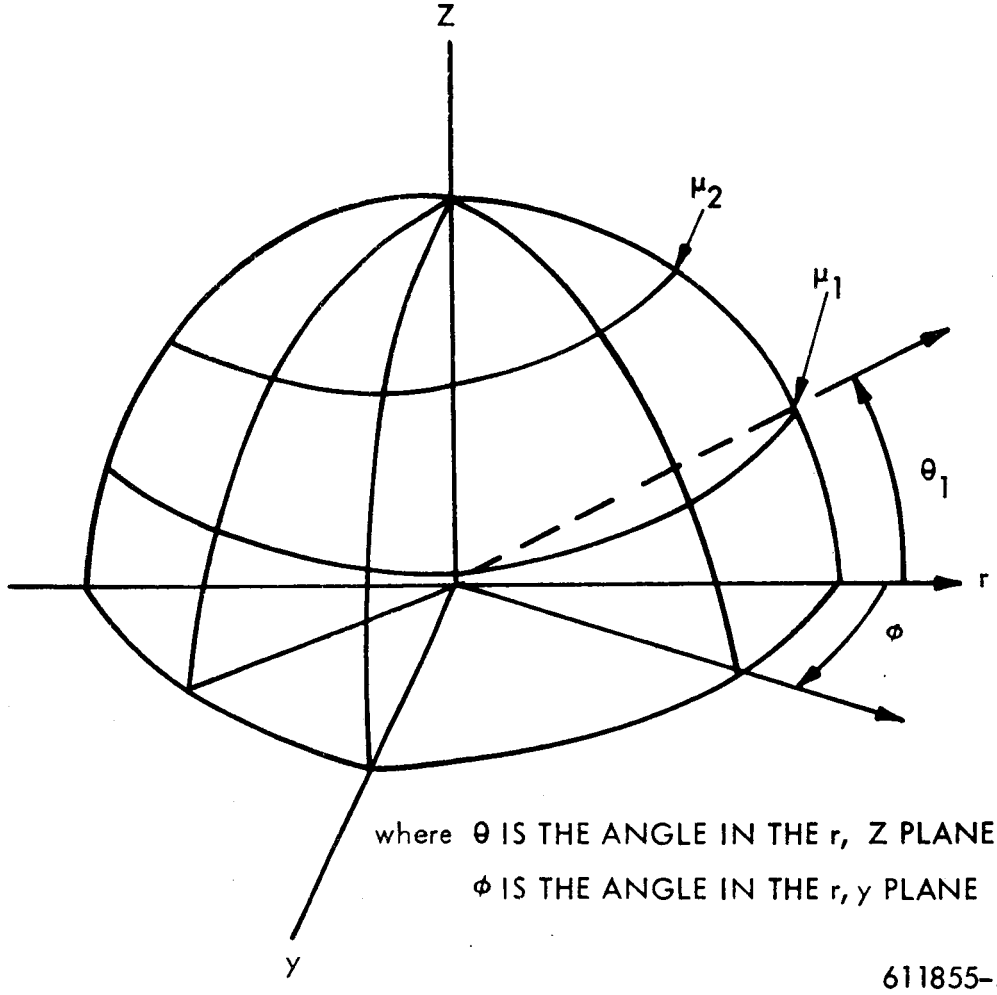


Figure 4. MIST, MISPHT, and TOPIC Angular Segmentation

b) If β_{bg} is some number in the interval (0, 1), then the fraction β_{bg} of any flux emerging from the boundary surface will be reflected back into the surface isotropically. For example, the current reentering the boundary surface will be exactly β_{bg} times the current leaving the surface, but the angular flux distribution reentering the surface is isotropic. $\beta_{b,g}$ is termed the "isotropic albedo coefficient".

c) The term $\gamma_{lbg} P(l)$ is a Legendre polynomial representation of an axially symmetric (no ϕ dependence) source at boundary b for group g. For convenient reference, if $\gamma_{lbg} = 0$ for $l \geq 1$, an isotropic entrant flux $N(x, \mu) = \gamma_{obg}$ will result, and the entrant current in this case will be:

$$\int_0^{2\pi} d\phi \int_{\Delta\mu_b} \gamma_{obg} \mu \, d\mu = \pi \gamma_{obg}$$

If an anisotropic source is specified (i.e., $\gamma_{lbg} \neq 0$ for some l), the program user should be sure that the Legendre polynomial coefficients have the correct sign for the odd values of l. The Legendre polynomial defines a flux distribution for both halfspaces of μ, and the flux distribution of an anisotropic source containing non-zero coefficients for odd values is not the same in both μ halfspaces; i.e., it is not symmetric about $\mu = 0$. The program user should make certain that the polynomial produces the desired flux distribution in the halfspace $\mu = 0$ to 1 when the source is applied at the left boundary and in the halfspace $\mu = -1$ to 0 when the source is applied at the right boundary.

d) The term $\Delta_{bg}(x_b, \mu)$ in the boundary condition equation permits application of a fixed boundary source. The program interprets this input flux distribution in the same manner as those fluxes it calculates internally; i.e., the flux distribution $\Delta_{bg}(x_b, \mu)$ will be assumed linear in each interval of the μ halfspace. (These intervals are defined, of course, by the μ space partitioning in which each halfspace is divided into intervals.) The program user defines this type of boundary condition by specifying point values of the desired flux distribution at each boundary for each group. In this way, output fluxes from one MIST or MISPHT problem can be

input directly to a new problem if both solutions have the same value of quadrature order n.

The boundary condition at either boundary (right or left) for each group in TOPIC can be expressed by the equation:

$$N_g(r_b, \mu, \phi) = a_{bg} N_g(r_b, \mu, -\phi) + \sum_{l=0}^{1} \gamma_{lbg} P(l)\left[\sqrt{1-\mu^2}\cos\phi\right] + \frac{\beta_{bg}}{C} \int_{\Delta\phi'} \int_{-1}^{1} \sqrt{1-\mu^2}\cos\phi\, N_g(r_b, \mu, \phi')\, d\mu\, d\phi' + \Delta_{bg}(r_b, \phi)$$

The constants a_{bg}, β_{bg}, γ_{lbg}, are identical to the MIST and MISPHT description except that the input values are in the angle ϕ instead of θ.

The range of μ is -1 to 1. However, when b is the right boundary, the range of ϕ is $-\frac{\pi}{2}$ to $\frac{\pi}{2}$, and the range of ϕ' is $\frac{\pi}{2}$ to $\frac{3\pi}{2}$; and when b is the left boundary, the range of ϕ' is $-\frac{\pi}{2}$ to $\frac{\pi}{2}$, and the range of ϕ is $\frac{\pi}{2}$ to $\frac{3\pi}{2}$.

The constant C is defined by the formula,

$$C = (-1)^S 4 \sum_{k=1}^{K} h_k \sqrt{1-\mu_k^2} = \int_{\Delta\phi'_S} \int_{1}^{-1} \sqrt{1-\mu^2}\cos\phi'\, d\mu\, d\phi',$$

where the exponent S is 1 for the right boundary, and 2 for the left boundary. The integral over the range of μ is approximated by Gauss quadrature.

The reason for the approximate calculation of C is that, in the TOPIC code, all integrals over the range of μ are calculated in this manner, including the integral which appears in the β_{bg} term. It is necessary to compute C in this manner to prevent the generation of a fictitious source of particles. When $\beta_{bg} = 1.0$, then C/π, instead of 1.0, times the outward current is reflected back, thus causing an erroneous source.

At the outer boundary in TOPIC, it is unrealistic to apply a symmetry condition using a_{bg} especially in neutron reactor cell problems, because application of the symmetry condition results in an angular flux of zero for $\phi = \frac{\pi}{2}$; i.e., $N(r_b, \mu, \frac{\pi}{2}) = 0$.

An option in the TOPIC program permits a more realistic use of the symmetry condition at the outer boundary. When $a_{bg} \neq 0$, and the input quantity MFR > 0, the TOPIC program sets the right boundary flux $N(r_b, \mu, \frac{\pi}{2})$ equal to a non-zero value[8].

The Legendre polynomial representation of a source at a boundary leads to difficulties in the TOPIC program. This source is axially symmetric about the radius vector. It should be noted that the application of Gauss quadrature for integration over the range of μ does not allow an exact prediction of the number of particles entering a surface in unit time and unit area for a given set, γ_{obg}, and γ_{1bg}. However, in the case when only the Legendre polynomial source on the right hand side of equation 2.10 is non-zero, the current into the surface produced by a given set, γ_{obg} and γ_{1bg} will be only slightly in error in the γ_{1bg} term.

The values input for $\Delta_{bg}(r_b, \phi_l)$, at each ϕ mesh point, are interpreted in the same manner as are all other functions in TOPIC; i.e., all integrations are performed with the assumption that the variation of Δ_{bg} between ϕ mesh points is linear with respect to cos ϕ.

2.2.7 Transverse Leakage Approximation

To account for the flux leakage in the transverse direction of the one-dimensional slab (MIST) or cylinder (TOPIC) geometry subprograms of TAPAT, a simplified transverse leakage correction is allowed. This correction factor ($DgBg^2$) is assumed to be an absorption in all calculations. If the program user specifies a transverse leakage correction, the total (or transport corrected) cross section for each region mixture and each group will be corrected by the quantity $DgBg^2$. The quantity $\Sigma_g^t + DgB_g^2$ appears in printed output data as the total cross section. All region and system neutron or photon energy balance calculations will include the total transverse leakage term as part of the group or total absorption term.

The transverse leakage correction is calculated as follows:

In slab geometry:

$$DgBg^2 = \left[\frac{1.0}{3.0^* \Sigma_g^t}\right]\left[\left(\frac{\pi}{Z^*}\right)^2 + \left(\frac{\pi}{Y^*}\right)^2\right]$$

or:

$$DgBg^2 = \left[\frac{1.0}{3.0^* \Sigma_g^t}\right]\left[\left(\frac{2.405}{R^*}\right)^2\right]$$

In the cylindrical geometry, the transverse leakage in the axial (Z) direction is given as:

$$DgBg^2 = \left[\frac{1.0}{3.0^* \Sigma_g^t}\right]\left[\left(\frac{\pi}{H^*}\right)^2\right]$$

where

Dg is the diffusion coefficient in group g defined as $\dfrac{1.0}{3.0^* \Sigma_g^t}$

Bg^2 is the total transverse direction buckling in group g.

Σ_g^t is the total (or transport corrected) collision cross section for the region mixture in each region for group g.

Z^*, Y^* are the two extrapolated transverse dimensions in rectangular geometry in the planes normal to the direction of the multigroup flux solution.

R* is the extrapolated transverse dimension in cylindrical geometry in the plane normal to the Z axis direction of the multigroup solution.

H* is the extrapolated transverse dimension in cylindrical geometry in the direction normal to the radial midplane where the radial midplane is the direction of the multigroup solution.

The above transverse dimensions (designated by asterisks) are the total extrapolated dimensions in a direction normal to the direction of the flux solution. The program user may input an actual transverse dimension, a single group independent value of the transverse direction, or provide input data to allow calculation of a group dependent extrapolated dimension Z* as follows:

$$Z^* = Z + d, \text{ or:}$$

$$Z^* = Z + \left[C^* \lambda_g^t \right]$$

where

Z^* = the value of the transverse dimension used in the transverse leakage term.

Z = the input value of the transverse dimension.

d = the extrapolation distance

C = the constant, 1.42089, used in the definition of extrapolation distance, d, from the transport relaxation length λ^t.

λ_g^t = the transport relaxation length defined in TAPAT as $\frac{1.0}{\Sigma_g^t}$

The calculation of each of the other transverse dimensions (Y*, R*, H*) are solved in an identical manner as Z* with the substitution of the input values Y, R, or H.

If the program user does not want an extrapolation distance, d, added to the input value of X, Y, R, or H; then the constant C is entered as zero.

If the user specifies a void region withall $\Sigma_g^t = 0.0$ or a group with $\Sigma_g^t = 0.0$, then the transverse leakage term is not computed for that region or group. However, if a region in a problem contains only a small atom density of a mixture (i.e., small Σ_g^t), then the use of a transverse leakage correction may lead to erroneous results since the group diffusion coefficients Dg will become large. The program user must, therefore, use discretion in the use of the transverse leakage correction.

2.3 MULTIGROUP SOLUTION IN THE DIFFUSION OR TRANSPORT THEORY PROGRAM

2.3.1 Energy Group Coupling

The solution of the multigroup set of diffusion or transport equations in each of the subprograms of the TAPAT system is described here. The diffusion subprogram ADDICT assumes only isotropic events (e.g., isotropic scatter-transfer of neutrons) and the energy group coupling is identical to the other TAPAT programs. The transport subprograms each allow up to a first order Legendre polynomial representation of the scattering function for scattering within a given energy group. While scattering from one group to another group, the scattered angular distribution is assumed to be isotropic.

Energy groups are coupled by:

1) scattering from a higher energy group into lower energy groups (i.e., downscatter),

2) scattering from lower energy groups into higher energy groups (i.e., upscatter),

3) and in neutron reactor problems, by fission, which produce source neutrons simultaneously in a number of groups.

All forms of coupling are described by the equation for the source terms q(r) or $q(r,\mu)$ in equations 2.1 and 2.3. The source is assumed to be isotropic in the transport programs; (i.e., $q(r) = q(r,\mu)$) and in any group the source is given by:

$$q_g(x) = \sum_{g'' \neq g} \Sigma^{s_o}_{g'' \to g}(x)\, N_{g''}(x) + \frac{\chi_g}{\lambda} \sum_{g'=1}^{NGR} \nu_{g'}\, \Sigma^{f}_{g'}(x)\, N_{g'}(x) + Q_g(x)$$

where:

$N_{g'}(x)$ is the usual scalar flux at the mesh point coordinate x (or r in cylindrical or spherical geometries), from the previous outer iteration.

$N_{g''}(x)$ is the scalar flux as calculated from a previous outer iteration in upscatter transfer or from a previous group solution in the same outer iteration in a downscatter transfer.

$\Sigma^{s_o}_{g'' \to g}$ is the cross section for scattering of neutrons or photons from group g'' to group g.

χ_g is the fraction of fission neutrons released in group g. In eigenvalue problems:

$$\sum_{g=1}^{NGR} \chi_g = 1.0$$ is normally used.

$\nu_{g'}$ is the number of neutrons produced per fission by neutron fission event in group g'.

$\nu_{g'}\ \Sigma^{f}_{g'}$ is the neutron fission production probability for neutrons in group g' which is formed by the product of the fission cross section multiplied by the number of neutrons per fission event.

NGR is the total number of groups.

λ is equal to unity in those problems which are not eigenvalue problems (i.e., fixed source problems). During the outer iterations of an eigenvalue problem, it is the computed eigenvalue from the last iteration.

$q_g(x)$ (particles/cm^3 sec) is the fixed volume source for group g. It remains constant throughout any problem, and is either a pointwise function of x or a boundary value.

2.3.2 Outer Iteration Cycle

There are five types of problems which may be solved with the TAPAT program. These are:

Type A: An eigenvalue problem with no fixed (distributed or boundary) sources.

Type B: A fixed (distributed or boundary) source problem with no fissions.

Type C: A fixed (distributed or boundary) source problem with fissions.

Type D: A concentration search problem where a specified concentration is varied until a desired eigenvalue is reached.

Type E: A region thickness search problem where a specified region thickness is varied until a desired eigenvalue is reached.

Problem types A, C, D, and E require outer iterations.

A description of the outer iteration cycle in the ADDICT, MIST and MISPHT subprograms are described first and only the features of TOPIC which differ from the other TAPAT subprograms are described in the second part of the discussion.

For these cases, a fission density P at point i is defined as:

$$P_i = \sum_{g=1}^{NGR} \nu_g \Sigma_{gi}^f N_{gi}$$

where the i subscript denotes values at the mesh point x_i (or r_i).

In problem type A, at the beginning of each iteration, the fission density P_i is normalized so that its integral over volume is some input value, FAC. Then, at the end of the iteration, the value of P_i is obtained at each point x_i over the total volume, v. The eigenvalue is then defined as:

$$\lambda = \left[\int_v P_i \, dv \right] / FAC$$

The fission density is then renormalized by dividing each new P_i by λ.

At this point a test for convergence is made. The problem may be made to converge pointwise or on the problem eigenvalue. If eigenvalue convergence is desired, the test is as follows:

$$\frac{\lambda_k - \lambda_{k-1}}{\lambda_k} < \text{EPS 1}$$

where k indicates the present iteration, k-1 the previous iteration and EPS 1 is an input quantity of convergence criteria. If the test is satisfied the problem is converged. If pointwise convergence is desired, each point value of the normalized fission density for a given iteration is divided by the respective normalized point value of the fission density of the previous iteration. Let E_{max} be the maximum value of this ratio and E_{min} be the minimum value of this ratio. Then the pointwise convergence test is:

$$\frac{E_{max} - E_{min}}{E_{max}} < \text{EPS 1}$$

If the test is satisfied, the problem is converged.

Fission density extrapolation at each point x_i may be applied after the third iteration. The extrapolation equation has the following form:

$$P_i^{k+1} = P_i^k (1.0 + \theta) - \theta P_i^{k-1}$$

where k is the number of the present iteration, and k-1 is the number of the previous iteration. The value θ is an input extrapolation constant.

Problem type B requires only a single outer iteration and no eigenvalue is computed.

In problem type C, the same procedure is followed except that the fission density is not renormalized after each iteration, an eigenvalue is not computed, and no extrapolation is allowed. Either pointwise or total integrated fission source convergence may be used with problem type C. The convergence test of problem type C is based on λ being the total integrated source from fissions.

For problem type C, the program user should make sure that the total neutron multiplication factor of the system is less than 1.0; otherwise, the problem will not converge.

In problem types D and E, outer iterations are required to converge eigenvalue and search variables. The search operations in TAPAT are controlled by the two convergence criteria EPS 1 and EPS 3. In addition, the input KIT 1 controls the maximum number of outer iterations performed between each search move to a new concentration or thickness. The eigenvalue convergence test is identical to the test described above. The search variable convergence test is as follows:

$$\frac{V_k - V_{k-1}}{V_k} < \text{EPS 3}$$

Both the eigenvalue and search variable convergence tests must be satisfied for the program to complete the outer iteration cycle.

If eigenvalue convergence is achieved before the maximum number of intermediate iterations (specified by KIT 1) is reached, the program computes the next search concentration of thickness. Conversely, if search variable convergence is achieved without eigenvalue convergence, the program continues the outer iteration cycle while rechecking the computed search variable after each KIT 1 outer iterations.

The outer iteration cycle in TOPIC is more complex since the angular flux solution is dependent upon the problem input data.

Certain TOPIC problems require only one outer iteration. These problems contain: (1) no fission density calculation in any region, (2) only one Gauss point in the angular quadrature of μ, (3) no anistropic scattering within any group (all $\Sigma^{S0}_{g \rightarrow g} = 0.0$), and (4) no mirror reflection at the right boundary (all $\alpha_{bg} = 0.0$).

In addition, the requirement of scalar flux convergence at each mesh point can be specified in TOPIC. The complexity of the outer iteration cycle convergence tests will not be described here except to note that similar logic as developed in the other TAPAT subprograms has been used in TOPIC.

The requirement of outer iterations in TOPIC to converge angular fluxes for certain types of problems has led to the use of the sign of the input value EPS 1 as a conditional test. If the value of EPS 1 is negative, no eigenvalue or fission density is calculated and the outer iteration cycle is continued for the specified maximum number of outer iterations or until the scalar flux is converged.

2.3.3 Search Operations

The concentration and region thickness search calculation in the TAPAT program system are identical in the calculation of new variable values. The following discussion is limited to region thickness (ΔR) searches, and the optional concentration search calculation. The search technique is based on a Lagrangian interpolation technique using the search variable values as a function of adjacent search outer iteration eigenvalues. The interpolation calculation for the region thickness ΔR for the specified region follows as:

$$\Delta R_{k+1} = \Delta R_k \frac{(\lambda - \lambda_{k-1})(\lambda - \lambda_{k-2})}{(\lambda_k - \lambda_{k-1})(\lambda_k - \lambda_{k-2})} + \Delta R_{k-1} \frac{(\lambda - \lambda_k)(\lambda - \lambda_{k-2})}{(\lambda_{k-1} - \lambda_k)(\lambda_{k-1} - \lambda_{k-2})} + \Delta R_{k-2} \frac{(\lambda - \lambda_k)(\lambda - \lambda_{k-1})}{(\lambda_{k-2} - \lambda_k)(\lambda_{k-2} - \lambda_{k-1})}$$

where the subscripts k, k-1, k-2 denote the present and two previous search variable calculations and;

λ = the eigenvalue obtained at the outer iteration immediately preceding each search variable calculation. The unsubscripted λ is the desired eigenvalue of the search calculation.

ΔR = the region mesh interval thickness.

In the first set of outer iterations the program uses the input value of ΔR for the specified region. At the completion of the specified number of outer iteration (input value KIT 1), or at the converged outer iteration, the program selects the input guess of region thickness, SGES, as the new region mesh interval thickness ΔR. This value is used in the next set of outer iterations until KIT 1 iterations or eigenvalue convergence is achieved. At this time a linear extrapolation of the region thicknesses (input, and the first guess) versus eigenvalue is used to calculate a third guess of ΔR. On the fourth and succeeding search calculations, the Lagrangian interpolation technique described above is used.

If on any search calculation, a negative value of ΔR_{k+1} is obtained the program logically selects ΔR_{k+1} as either a factor of 5.0 or 0.2 times one of the previous variable values, ΔR_k or ΔR_{k-1}. This procedure uses the slope of the search value curve to determine which factor (i.e., 5.0 or 0.2) is applied to either ΔR_k or ΔR_{k-1}. The search calculation then proceeds in the normal fashion.

2.4 DATA PROCESSING PROGRAM: FLUX EDIT

The data processing subprogram (FLUX EDIT) in the TAPAT program system contains four separate routines. The purpose of each of the four routines in FLUX EDIT is:

1. Fixed source generation routine: Calculates and properly places multigroup distributed fixed sources in TAPAT regions from input spatial and energy distributions.
2. Flux Edit Routine: Calculates multigroup neutron or photon energy flux reaction rates (e.g., capture rates, energy deposition, dose rates, etc.); performs region integrals and spatial distribution normalization; and calculates source in TAPAT regions on an individual mesh point basis.
3. Pause Routine: Provides a program stop to allow the computer operator to change or mount a master cross section tape between linked TAPAT problems.
4. Punch Routine: Provides a punched decimal data deck of reaction rate distribution data and mesh point coordinates.

The primary purpose of the FLUX EDIT subprogram is to allow the TAPAT user to run a series of TAPAT problems in succession to obtain a complete radiation analysis in a single problem set. Consider the problem of calculating neutron and photon energy flux distributions at the radial midplane in a cylindrical reactor. Assume that neutron fission density distribution is known from a previous problem and that a complete radiation analysis is to be performed. This analysis is a five-step process:

1) The fixed source generation routine is used to calculate the distributed fixed neutron source from the input neutron fission density.

2) The neutron transport calculation is performed in TOPIC to obtain multigroup neutron flux distribution.

3) The flux edit routine is used to calculate neutron reaction rates including distributed fixed photon energy sources.

4) The photon transport calculation is performed in TOPIC to obtain multigroup photon flux distribution, and,

5) The flux edit routine is used to calculate photon reaction rates.

This five-step process, though requiring a large amount of input data, is set up as a single TAPAT deck, but runs as a set of stacked problems in the TAPAT system.

The need for the FLUX EDIT routines is evident if one considers (1) the numerical solution of multigroup flux data in the TAPAT diffusion or transport programs, and (2) the data processing for linked TAPAT problems. The problem of definition of TAPAT mesh point indices illustrates a portion of the numerical solution. Flux mesh points correspond to the number of mesh points describing the reactor geometry. The total number of points at which fluxes are obtained is equal to the number of mesh intervals plus one. Since the TAPAT program system solves for fluxes at each flux mesh point, there exist two values of fission density, reaction rate, or fixed source values at each internal region boundary. The number of fission density, reaction rate, fixed sources then depends upon the number of regions and mesh points. Therefore, a source mesh point number is related to the flux mesh point number and the region number as:

$$j = i - 1 + m$$

where

j = a source mesh point number

i = a flux mesh point number

m = a region number

The index j then includes the double values required at each internal boundary in a TAPAT problem.

The fixed source generation routine in the FLUX EDIT subprogram of TAPAT employs a simplified technique of inputting distributed fixed sources into TAPAT problems. The fixed sources required for a TAPAT problem consist of multigroup data at each mesh point in a region. This multigroup mesh point data, Q_{ig}, is assumed in the fixed source generation routine to be separable into a spatial distribution F_i and an energy spectrum, Γ_g. The fixed source then follows as:

$$Q_{ig} = F_i * \Gamma_g$$

The data for a fixed source generation problem is illustrated in the following example.

Consider a three region problem as shown in Figure 5. The fixed source data in each region consists of groupwise data at mesh points 1, 2, 3 for region number 1, mesh points 3, 4, ..., 10 for region 2, and mesh points 10, 11, 12 for region 3. The fixed sources at the internal region boundaries between regions 1 and 2 and regions 2 and 3 require a double value (i.e., a fixed source representative of the region material on each side of the boundary). These double values are required since the solution of fluxes occurs at the mesh points in the TAPAT programs.

The TAPAT programs account for the double values at each internal region boundary. For example, the number of fixed value sources required for the problem shown in Figure 5 is 15 values, where the values at 1, 2, and 3 are for Region 1; the values at 4, 5, ... 11 are

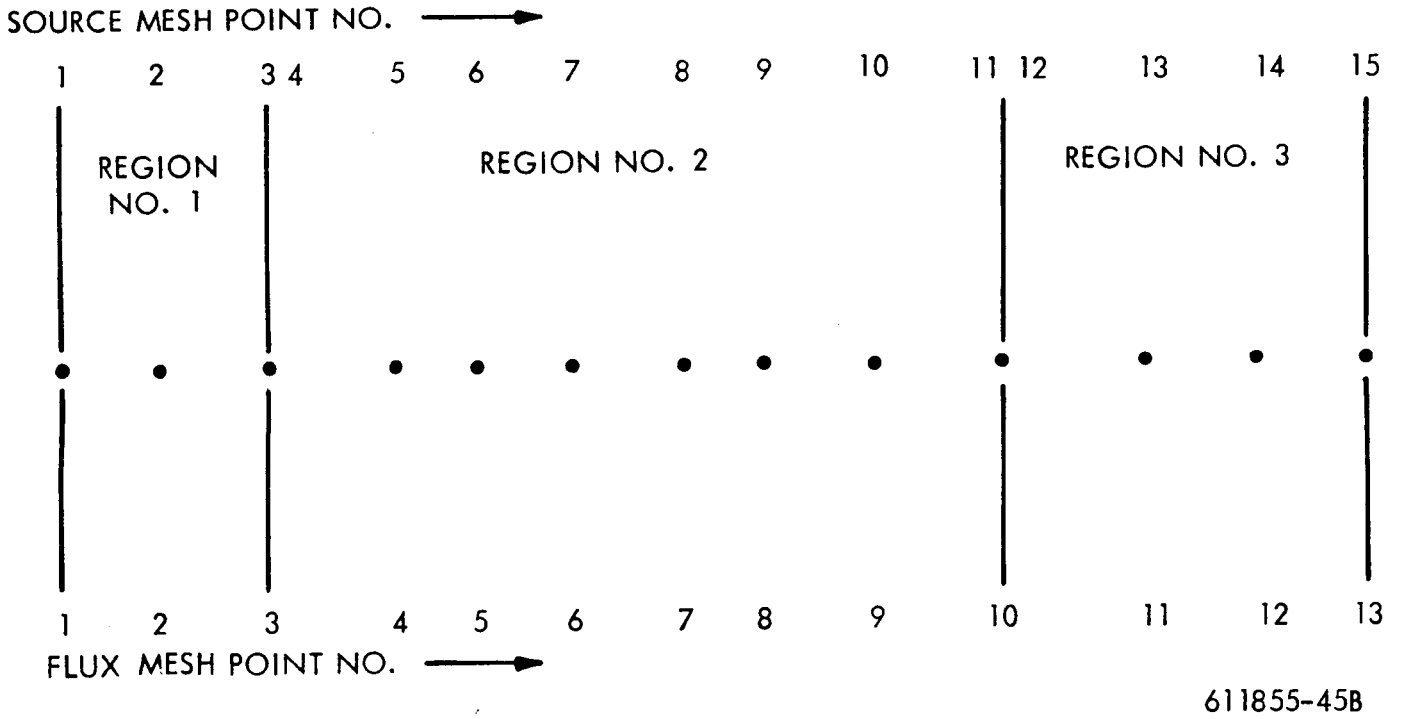


Figure 5. Flux and Mesh Point Numbering System

for region 2; and the values at 12, 13, 14, and 15 are for Region 3. The source values at points 3 and 4, and points 11 and 12 are calculated for the groupwise fluxes at the flux mesh points 3 and 10, respectively.

The flux edit routine in the FLUX EDIT subprogram of TAPAT is a data processing routine. The operations performed in this routine can be discussed in a general manner if one considers a group reaction rate at a mesh point to be the group response value times a flux value. The total reaction rate is then the summation over all groups in the multigroup solution.

The operation to be performed in the flux edit routine is controlled by input control data. The initial operation in the flux edit is the calculation of the following:

Group source mesh point reaction rate:

$$RR_{jg} = F_{mg} * N_{ig}$$

where

RR_{jg} = the reaction rate in group g at source mesh point j.

F_{mg} = the response value for group g and the material m at the source mesh point j.

N_{ig} = the scalar flux in group g at mesh point i.

Total source mesh point reaction rate:

$$RR_{j} = \sum_{g=1}^{NGR} RR_{jg}$$

where

NGR = the total number of groups in the multigroup fluxes to be edited (e.g., the number of neutron groups).

These calculations for a single set of multigroup response values for each source mesh point j are a complete problem set. At the completion of the mesh point calculations, the integration of the reaction rate mesh point values is obtained as described in the following discussion.

The TAPAT programs solve for the fluxes at flux mesh points. Since the reaction rate (e.g., fissions, capture) is double valued at each internal region boundary mesh point, an integration routine is used for all integration calculations which have two volume elements or integration coefficients for each mesh point. This method is used for computational ease. The coefficients in each of the three geometries (slab, sphere, or cylinder) for the volume element ΔV_{ri} to the right of each flux mesh point and the volume element ΔV_{li} to the left of each flux mesh point follow as:

SLAB:

$$\Delta V_{ri} = \frac{X_{i+\frac{1}{2}} - X_i}{2.0}$$

$$\Delta V_{li} = \frac{X_i - X_{i-\frac{1}{2}}}{2.0}$$

CYLINDER:

$$\Delta V_{ri} = \pi \left[R^2_{i+\frac{1}{2}} - R^2_i \right]$$

$$\Delta V_{li} = \pi \left[R^2_i - R^2_{i-\frac{1}{2}} \right]$$

SPHERE:

$$\Delta V_{ri} = \frac{4}{3} \pi \left[R^3_{i+\frac{1}{2}} - R^3_i \right]$$

$$\Delta V_{li} = \frac{4}{3} \pi \left[R^3_i - R^3_{i-\frac{1}{2}} \right]$$

where subscripts $i + 1/2$ and $i - 1/2$ refer to the midpoint of the interval bounded by the mesh points i, $i + 1$, and $i - 1$, i. The values R are the mesh point coordinate dimensions in the slab, cylindrical or spherical problem.

The integration coefficients are used with each value of the reaction rate at a source mesh point to obtain region integrals. If one considers each region, m, (as described in TAPAT) as a set of equal sized mesh intervals bounded by the region boundary mesh points II_{m-1}

and $\ell\ell_m$ as shown in Figure 6, the region integral reaction rate, RR_m of the individual source mesh point reaction rates RR_i follows as:

$$RR_m = \left[\sum_{i=\ell\ell_{m-1}}^{\ell\ell_m - 1}\right] \Delta V_{ri} * RR_i + \left[\sum_{i=\ell\ell_{m-1}+1}^{\ell\ell_m}\right] \Delta V_{\ell i} * RR_i$$

The index on source mesh point, j, is internally calculated from flux mesh point indices and region numbers as described previously. In addition, the cross sectional area, thickness, or volume of each region is obtained in a similar fashion as:

$$V_m = \left[\sum_{i=\ell\ell_{m-1}}^{\ell\ell_m - 1} \Delta V_{ri}\right] + \left[\sum_{i=\ell\ell_{m-1}+1}^{\ell\ell_m} \Delta V_{\ell i}\right]$$

At the completion of the integration of a single reaction rate in all regions of the TAPAT problem, the integral reaction rate, RR_m, for region m is used with the volume V_m, (i.e. cross sectional area in cylinder, region thickness in slab, volume in sphere) of the region to calculate the average reaction rate as:

$$\overline{RR}_m = \frac{RR_m}{V_m}$$

This average value $\overline{RR}_m$ is then used to calculate the normalized reaction rate as:

$$RR'_i = \frac{RR_i}{\overline{RR}_m}$$

where

RR'_i = the normalized reaction rate such that the area weighted average is one.

When the region calculations are completed, the program can calculate each source mesh point spectrum from the specific reaction rate data as:

$$Q_{ik} = \chi_k * RR_i$$

where

Q_{ik} = the neutron or photon energy source in group k at source mesh point j.

x_k = the neutron or photon energy release in each group k from the specific reaction rate calculated.

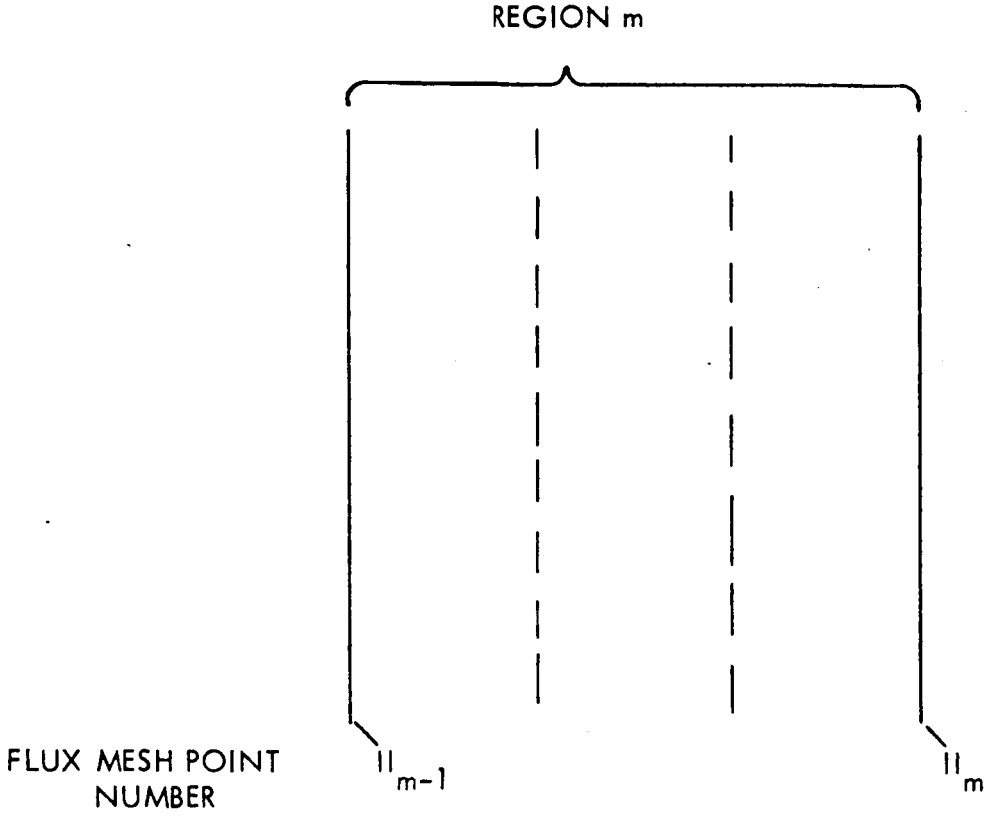
This source data, Q_{ik}, can be accumulated over all reaction rate calculations (e.g., photon production neutron reactions of fission, capture, inelastic scatter) in a FLUX EDIT data deck. This accumulated source data is then available in TAPAT for a photon transport problem.

For example, the POINT program as described in Volume 2 of this report, prepares a flux edit input data deck to be used intermediate to a neutron and a photon transport problem in TAPAT. This deck contains as separate flux edit problems the following: reaction rate response values for calculating the neutron energy deposition reaction, and the photon production for neutron reactions of radiative capture, fissions, and inelastic scatter.

As a special feature in the flux edit routine, the program user can obtain printed source distribution data for use in point kernel analyses. With the neutron or photon source spectrum at each mesh point, the flux edit program will integrate this data (i.e. obtain a summation over groups) and obtain for each region the integrated source spectrum, the normalized distribution, and the average source spectrum. These data are then printed as output for flux edit along with the calculated neutron or photon source at each source mesh point.

The pause routine in FLUX EDIT is a programmed stop which prints an on-line comment, "PLEASE PERFORM OPERATIONS AS REQUESTED ON YELLOW CARD AND HIT START". The IBM 7094 operator should follow instructions on the job submittal card and hit the start button on the 7094 console.

The punch routine in FLUX EDIT provides the program user with a means of punching (in TAPAT floating point input card format) the calculated data in specific core memory locations. This routine punches the reaction rate data calculated by flux edit for use in plotting routines. Included in each reaction rate punched data is the flux and source mesh point coordinate dimensions as two separate decks of punched output.



II_{m-1} AND II_m ARE RIGHT BOUNDARY MESH POINT NUMBERS FOR THE mth-1 AND mth REGIONS IN A TAPAT PROBLEM.

611855-48B

Figure 6. Schematic Diagram of a TAPAT Region

SECTION

3.0 INPUT DATA DESCRIPTION

3.1 GENERAL DESCRIPTION

The input of each TAPAT problem requires four types of data in the following order:

Type 1 - Selection of the program within the TAPAT System, e.g., ADDICT, MISPHT, MIST, TOPIC, or FLUX EDIT (control card).

Type 2 - Title card or problem description (alphanumeric data).

Type 3 - Fixed point data.

Type 4 - Floating point data.

Additional problems (change cases) in the TAPAT system require as input each of the four types of data listed above; but only those data words which change from case to case are required input in Type 3 and 4 input. Each of the four types of input data is described in detail in Section 3.1.

3.1.1 Data Type 1 (Control Card)

This data transfers to the specific program of interest. The control word is placed in Column 2 of the control card.

Control Word	
0	Transfer to ADDICT Diffusion Theory program
1	Transfer to MISPHT (Sphere) S_n Transport Theory program
2	Transfer to MIST (Slab) S_n Transport Theory program
3	Transfer to TOPIC (Cylinder) S_n Transport Theory program
4	Transfer to fixed source generator routine
5	Transfer to FLUX EDIT routine
6	Pause 7777 to allow master cross section tape mounting
7	Transfer to punch routine

3.1.2 Data Type 2 (Title Card or Problem Identification)

This card may contain any desired alphanumeric information in columns 1 - 70. A "1" punch in column 1 will start all on-line and off-line printouts at the top of a new page. This card must be included in each problem. In order to initialize a problem properly, the last two columns (columns 71 - 72) are reserved for an input word. If columns 71 - 72 contain a 99 then all data storage locations are set to 0.0 and the problem data which follow must be a complete problem.

3.1.3 Data Types 3 and 4 - Fixed and Floating Point Data

The card format for the fixed point data is as follows:

Card Columns 1-2	Number of pieces of data on this card (right adjusted*) $1 \leq$ No. ≤ 21
Card Column 3	1 - this is the last fixed point data card: 0 - (or blank) this is not the last fixed point data card
Card Columns 4-8	Address of first piece of data on the card (right adjusted)
Card Columns 9 - 71	Up to 21 pieces of integer data (each right adjusted in FORTRAN format I3)

The card format for the floating point data is as follows:

Card Columns 1-2	Number of pieces of data on this card (right adjusted)
Card Column 3	1 - this is the last floating point data card 0 or blank - this is not the last floating point data card
Card Columns 4-8	Address of first piece of data on the card (right adjusted)
Card Columns 9-68	Up to six pieces of floating point data in Format 6E 10.5.

*"Right adjusted" means the last significant digit of a number is at the extreme right of a field.

Some valid ways of writing a floating point word in the ten column field are as follows for the number 3.1415:

				Card Columns					
1	2	3	4	5	6	7	8	9	10
+	3	1	4	1	5	0	+	0	0
3	.	1	4	1	5	0	+	0	0
3	.	1	4	1	5	E	+	0	0
3	.	1	4	1	5	0	0	+	0
3	1	.	4	1	5	0	0	-	1
.	0	3	1	4	1	5	0	+	2
(b)	3	.	1	4	1	5	0	+	0
3	1	4	1	5	0	E	+	0	0
3	.	1	4	1	5	0	0	(b)	(b)

(b) indicates a blank

The fixed or floating point data may be entered in any order and on as many cards as desired, so long as all fixed point data cards precede all floating point cards. The reading of types of data, fixed and floating, is terminated by a 1 in column three of the last fixed or floating point data card. The reading of data from each card of fixed or floating data is in sequence from the first data field (columns 9 - 11 for fixed and columns 9 - 18 for floating)

on the card. Data are assigned a specific address or location in core memory storage according to the address on the card and the data field in which the piece of data appears. For example, if a fixed point data card is input as follows:

Column No.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
		3					1	6		1	0		1	2		1	6			

the piece of data in Columns 15 - 17 (16 in Data Field 3) is assigned to Address 18. If the data card is set up wrong, such as a 2 in Column 2, the piece of data in Columns 15 - 17 (16 in Data Field 3) is not entered in Address 18 and the data in Address 18 is not altered. In using this card format and addressable input, it follows that zero values need not be entered. In addition, if the data in a specific address is not to be changed in a succeeding problem (a change case), these data need not be entered.

Pieces of data which are internally calculated or changed in the program must be input with each case. These data are noted in the following input description:

Blank data fields are considered zeros; hence, care must be taken to assure that the specified number of pieces of data in Columns 1 - 2 is the desired quantity; otherwise, zeros may be stored in locations where they are not wanted.

In order to run change cases, only those data words which are different from the preceding case need be entered. Caution should be exercised when running change cases because unwanted data from the preceding cases may be carried over. Every problem or case must have at least four cards; i.e., one problem selection card, one alphanumeric title card, one fixed-point data card, and one floating-point data card.

The POINT Program (Volume 2) calculates and punches on cards the neutron and photon cross section data for input to the TAPAT System. The POINT Program also punches data for input to the FLUX EDIT subprogram as discussed in Section 3.4.

3.2 PROGRAM ADDICT (DIFFUSION THEORY) INPUT DATA

The following table is a description of the input quantities pertaining to the diffusion theory program (ADDICT) in the TAPAT System. This program is selected if a zero is punched on the control card. The fixed and floating-point data are entered under standard TAPAT formats described in Section 3.1.3.

3.2.1 Fixed Point Data

Address	Name	Description
1	MAX	Total number of mesh points (number of intervals plus one) $3 \leq MAX \leq 100$
2	JMAX	Total number of regions $1 \leq JMAX \leq 30$ A TAPAT region is a set of consecutive mesh intervals with the same ΔX or ΔR, and same mixture cross section set. Hence, if a variable mesh is desired in a single physical region, more than one TAPAT region must be used to describe a physical region.
3	NGR	Total number of energy groups. $1 \leq NGR \leq 20$
4	NDS	Number of downscatter groups. $0 \leq NDS \leq 6$ The number of downscatter groups can be defined as one plus the maximum number of groups which can be skipped in scattering down from any group. It ranges from zero (no downscatter) to a maximum of 6 in TAPAT (e.g., Group 1 particles can scatter to Group 7). (See Table 1)
5	NPS	Number of upscatter groups. $0 \leq NPS \leq 5$ The number of upscatter groups can be defined as one plus the maximum number of groups which can be skipped in scattering up from any group. It ranges from zero (no upscatter) to a maximum of 5 in TAPAT (e.g., Group NGR particles can scatter to Group NGR-5). (See Table 1).
6	NOT*	Output control word. If NOT has a negative sign, the program punches fission density and group fluxes as TAPAT addressed decimal data cards and if punched data is desired for each problem of a set of TAPAT problems, NOT must be a negative number for each problem.

* Input words with an asterisk are not the same in the transport theory codes. All other words are identical in both the diffusion and transport theory codes.

Address	Name	Description
		NOT = 0 - print eigenvalue, fluxes, and fission density. NOT = 1 - print above information plus region and system balance characteristics.
7	IG*	Geometry control word for solution of eigenvalue, fluxes, and fission density. IG = 0 - slab geometry solution. IG = 1 - cylinder geometry solution. IG = 2 - sphere geometry solution.
8	ITOUT	Number of outer iterations; ITOUT = 0 specifies a single outer iteration. Maximum number of outer iterations is set to 50 unless otherwise specified. For a fixed distributed or boundary source problem, iterations are required only when fissionable materials are present and iterated fission density is desired. When NOT > 0 then ITOUT + 1 outer iterations (as a maximum) are done to store extra data needed for output edits.
9	LCO	Fission density convergence option. LCO = 0 - pointwise fission density convergence. LCO = 1 - eigenvalue (or total iterated fission density in a fixed source calculation) convergence.
10	NMIX	Number of pieces of data in the mixture vector.** (Equal to length of MIX or CONC vector.) $0 \leq NMIX \leq 80$ See explanation of the input data MIX and CONC, as well as Section 3.5 for details.
11	MMIX	Number of cross-section sets (elements, isotopes, or materials) to be read from the master cross-section tape. This master tape is mounted on the MSFC IBSYS Version 13 Unit B-6. $0 \leq MMIX \leq 20$

** Note: The word vector is commonly used to describe a list of data.

Address	Name	Description
12	MUTEST*	Diffusion coefficient (D_g or floating point data DIFE) option:

MUTEST = 0 - diffusion coefficients by group for the mixture cross section set in each region m (i.e., MIR_m) must be input with the mixture cross section set data.
MUTEST = 1 or 2 - diffusion coefficients for the mixture cross section set in each region m (i.e., MIR_m) are calculated from the macroscopic total or transport cross section Σ^t_g, in each group and the macroscopic absorption cross section, Σ^a_g, in each group as:

$$D_g = \frac{1.0}{3.0 * \Sigma^t_g} \quad : \text{MUTEST} = 1, \text{ or}$$

$$D_g = \frac{1.0}{3.0 * \kappa^2 * \Sigma^t_g} \quad : \text{MUTEST} = 2, \text{ where}$$

$$\kappa = 1.0 - \left[\frac{2.0 * \Sigma^a_g}{5.0 * \Sigma^t_g}\right]$$

Note: When MUTEST is equal to 1 or 2, the macroscopic cross section data in each region (assigned by the input data MIR_m) must be a calculated mixture of cross section data from the mixture operations specified in the MIX and CONC data values.

13	IDP	Input data print option

IDP = 0 - print input data
IDP = 1 - do not print input data

14	JSP	Search calculation option.

JSP = 0 - no search calculation, but perform an eigenvalue, distributed fixed source, or boundary fixed source calculation.
JSP = 1 - concentration search calculation.
JSP = 2 - zone thickness search calculation.

Address	Name	Description
15	LPG	Fission density input guess option LPG = 0 - flat guess, normalized to the input floating point data value, FAC. LPG = 1 - input pointwise guess with the integral normalized to the value, FAC. LPG = 2 - fission density guess from previous TAPAT problem preceding this problem (data still in memory core storage). The integral normalized to value, FAC. This word has no meaning if there are fissionable regions in a problem. In a distributed or boundary fixed source problem with no fissions, the fission density guess is set equal to zero for all mesh points.
16-45	II	Upper right (boundary) mesh point number for each region. Each region must have at least one interval. The first left boundary of a TAPAT problem is mesh point Number 1. (Each TAPAT region has a constant ΔR or ΔX within the region.)
46-75	MIR	Mixture cross section set number of the macroscopic cross section data which is to be used in each region; data are entered for Region No. 1 to Region No. JMAX. Mixture numbers are in reference to the mixtures formed in the MIX vector or addressed input macroscopic cross section data. Each region must have a mixture number specified. (See Section 3.5 for details.)
76-155	MIX	Mixture or material cross section set numbers to specify the cross section mixtures to be formed. Each element of the mixture vector is a mixture or material number. The respective concentration, which is a volume fraction or atom density, is entered in the CONC vector (floating point data). Mixture number is given first and the constituent material numbers follow. In the CONC vector, a mixture number is designated by a zero; hence, constituent material CONC's must be non-zero. The maximum length of the mixture vector is 80; therefore, NMIX $\leq$ 80. (See Section 3.5 for more details.)
156	N*	Buckling (B^2) input option: Values of B^2 are entered in one of two sets of floating point data locations dependent upon the value of N. 1 - A single value of B^2 for all regions or groups is entered in floating point Address 12011.

Address	Name	Description
		2 - A set of group values of B^2 for all regions are entered as NGR values in Addresses 12011 to 12011 + NGR-1. 3 - A set of region values of B^2 for all groups are entered as JMAX values in Addresses 12011 to 12011 + JMAX-1. 4 - A complete set of region and group values of B^2 are entered in the appropriate Addresses 11411 to 12010.
157	MIK*	Extrapolated boundary condition for group fluxes. Calculations are performed using values of β_g which are obtained as a function of the region properties within that boundary. MIK = 1 - the values of β_g will be calculated internally to the program according to the equations in Section 2.1. MIK = 0 - β_g's = 0, or input values of β_g are entered by the user.
158-177	MTIX	Tape cross section set identification numbers to be read from the master tape. All identification numbers must appear in the same order in MTIX as they appear on tape. Maximum number of sets is 20, and MTIX's are consistent with the tape.
178-197	NTMIX	Mixture or material set numbers corresponding to the tape set numbers (MTIX) to place tape cross section sets in mixtures 1 - 30. The NTMIX set numbers permit the user to place a material or element cross section set from the master tape, designated by MTIX, in the set number, NTMIX. Maximum number of sets is 20, and the value NTMIX must be less than or equal to 30. (See Section 3.5 for more details.)
198	KREG	Region number, 1 through 30, to be used as the search zone thickness variable for the search option; JSP = 2.
199	NSOS	Position in mixture vector (1 through 80) of the material or mixture number and concentration to be the concentration search variable in the search option, JSP = 1. The value of NSOS specifies which material number, MIX, will be varied to achieve a desired eigenvalue. $2 \leq$ NSOS $\leq$ NMIX and NSOS not equal to a position with CONC = 0.0.
200	NFOS	Position in mixture vector (1 through 80) of the material or mixture number and concentration to be the concentration search filler variable in the search option JSP = 1. NFOS = 0 allows no substitution of a material or mixture for changes in the concentration search variable (NSOS) material. $2 \leq$ NSOS $\leq$ NMIX and NFOS $\neq$ NSOS.

201	KIT1	The number of outer iterations per search iteration. This allows the user to force new concentration or zone thicknesses search moves after each KIT1 outer iteration so that eigenvalue and search is converged simultaneously. $3 \leq KIT1 \leq 10$ and KIT1 = 3 or 4 recommended.
202	MFR*	No effect.

3.2.2 Floating Point Data

Address	Name	Description
1	EPS1*	Convergence criterion. EPS1 has meaning only if there is fissionable material in the problem. EPS1 is the convergence criterion on the pointwise fission density or integrated fission density. If LCO = 0: Pointwise convergence criteria of fission density must be met. If LCO = 1: Integral convergence criteria of fission density (eigenvalue) must be met.
2	EPS2*	Not applicable.
3	XIN	The value of the radius or dimension at the center or left boundary. This word specifies the value of the slab dimension, cylinder radius, or sphere radius at the left (center or inner) boundary. It need not be zero, but it cannot be negative. $0.0 \leq XIN$.
4	THETA	Power extrapolation factor to be used to accelerate outer iteration convergence. A value of 0.0 or 0.2 is recommended to avoid excessive over-extrapolation. A value of $\theta = 0$ (or blank) corresponds to no extrapolation. A value of $\theta > 0.2$ can cause divergence of the fission density. The extrapolation procedure on the fission density guess for the next outer iteration N + 1 from the Nth and N-1 iterations is as follows: $$P^{N+1} = P^{N}(1.0 - \theta) + P^{N-1}\theta.$$

Address	Name	Description
5	FAC	Fission density normalization factor. The total fission neutron source, F_t, which is calculated as: $$F_t = \sum_{g=1}^{NGR} \int_V \left(\nu_g \Sigma_g^f\right) N_g \, dV$$ is always used with FAC to obtain a value of the normalization parameter, FAC/F_t, and this value is used to multiply all fission density and flux values. FAC has no meaning in either a distributed or boundary fixed source problem. If no value for FAC is read in, it is automatically set equal to 1.0 by the program.
6	SGES	First guess of search variable modifier to be used in concentration or zone thickness search calculations. The value of SGES is the first modification of CONC or DELR, and the third and succeeding guesses are internally calculated by the program.
7-36	DELR	ΔR (or ΔX) specifications. The values of DELR are the interval widths ΔR (or ΔX) which are used in each TAPAT region. Each ΔR (or ΔX) must be greater than zero or an error indication will be printed.
37-636	SIGT	Total or transport cross sections by group and mixture*. This is the total collision (or transport corrected) cross section, σ_g^t, entered by group and mixture. Either macroscopic or microscopic cross sections may be read in; but since only macroscopic values are used by the program, any microscopic cross section sets should be multiplied by the proper atom densities (by use of the cross section mixing operation specified by NMIX, MIX, CONC). Cross sections for a given mixture can be read into the program without being used in any region of a given problem. This permits the user to read in

* A mixture cross section set is a macroscopic set of data which is used as a region material. Mixtures are composed of materials or elements, and may be input or internally calculated by the program.

Address	Name	Description

all the cross section sets for a series of problems in the first TAPAT problem. Then, one need only refer to the proper mixture numbers in the succedding change cases:

37 - 56 Mixture 1, Groups 1 - 20
57 - 76 Mixture 2, Groups 1 - 20
. .
. .
. .
417 - 436 Mixture 20, Groups 1 - 20
. .
. .
. .
617 - 636 Mixture 30, Groups 1 - 20

Specific cross section address = 36 + [(Mixture No. - 1)*(20)] + Group No.

637-1236 SIGS

Zeroth moment (P_o) scattering cross sections by group and mixture. This list of $\sigma^{S_0}_{g \rightarrow g}$ is for each mixture, the cross sections for isotropic (zeroth moment) scattering within each group. These cross sections are only those for nondegrading scattering (no down-scatter). Cross sections are stored identical to SIGT with beginning address at 637. Specific cross-section address = 636 + [(Mixture No. - 1)* (20)] + Group No.

1237-1836 SIGS1

First moment (P_1) scattering cross sections by group and mixture. This list of $\sigma^{S_1}_{g \rightarrow g}$ are, for each mixture, the cross sections for first moment non-degrading scattering (no down scatter) cross sections for scattering within each group. Cross sections are stored identical to SIGT with the beginning address at 1237. Specific cross section address = 1236 + [(Mixture No. -1)* (20)] + Group No.

1837-2436 VUSIG

Neutron fission cross sections by group and mixture. The list of $\nu_g \sigma^f_g$ is, for each mixture, the neutron production cross sections (number of neutrons per fission times the fission cross section) for each group. Cross sections are stored identical to SIGT with beginning address of 1837. Specific cross-section address = 1836 + [(Mixture No. - 1) * (20)] + Group No.

Address	Name	Description
2437-2456	CHI	Fission neutron spectrum: χ_g: $\sum_{g=1}^{NGR} \chi_g \equiv 1.0$ for eigenvalue problems. The quantity, χ_g, defines the fraction of fission neutrons released in each group. For all problems at least one non-zero CHI must be input. The final eigenvalue in a TAPAT problem without fixed sources (distributed or boundary) is based on neutrons in the system. $\sum_{g=1}^{NGR} \chi_g$
2457-5426	STR	Group to group transfer cross sections (downscatter) by mixture. This list of $\sigma^{S0}_{g' \rightarrow g}$ values is for each mixture, the cross sections for isotropic $g' \rightarrow g$ (zeroth moment) transfer of neutron or photon energy from each group to any of the lower energy groups. These cross sections govern the actual quantities of neutron or photon energy which are transferred by down-scattering from one group to any other (maximum of six-group down scatter). This list is a truncated list of data containing only the possible non-zero entries. The entry of specific cross sections is illustrated in Table 1. Specific cross section address = 2466 + [(Mixture No. - 1) * 99] + Cross Section position from Table 1.
5427-5876	STRU	Group-to-group transfer cross sections (upscatter) by mixture. This list of $\sigma^{S0}_{g \rightarrow g'}$ values gives, for each mixture, the cross sections for isotropic (zeroth moment) transfer of neutrons from each group to any of the higher energy groups. These cross sections govern the actual quantities of neutrons which are transferred by upscattering from one group to any other group (maximum of five group upscatter). These transfers are limited to the bottom six groups of a TAPAT problem. This list is a truncated list of data containing only the possible non-zero entries. The entry of specific cross section data is illustrated in Table 1. Specific cross section address = 5427 + [(Mixture No. - 1) * 15] + Cross Section position from Table 1.
5877-5916	ALPHA*	Boundary condition indicators: Left and right boundary condition indicators for each group, $ALPHA_{bg}$. $ALPHA_{bg}$ = 0.0 - extrapolated ^{bg} flux boundary condition using group ^{bg} dependent β_{bg}'s (TAPAT input BETA or internally calculated): $$N_{bg} + \beta_{bg}\left[\left(\frac{dN_g}{dr}\right)_b\right] = 0.0$$

Address	Name	Description

$ALPHA_{bg}$ = 1.0 - zero current boundary condition $\left(\frac{dN_g}{dr}\right)_b = 0.0$

$ALPHA_{bg}$ = 2.0 - zero flux boundary conditions: $N_{bg} = 0.0$

$ALPHA_{bg}$ = 3.0 - fixed boundary flux: $N_{bg} = \Delta_{bg}$

ALPHA's are initially set to 1.0 (left) and 0.0 (right) and need not be input if these conditions are desired.

5877 left boundary, Group No. 1
5878 right boundary, Group No. 1
5879 left boundary, Group No. 2
. .
. .
. .
5915 left boundary, Group No. 20
5916 right boundary, Group No. 20

5917-5956 BETA* Flux extrapolation parameters at left and right boundaries: If $ALPHA_{bg} = 0.0$; and if MIK = 0, the program calculates β_{bg}'s from equations in Section 2.1. Otherwise, the user must input β_{bg}'s if an extrapolated flux condition is desired.

BETA's are input in similar order as ALPHA's with a beginning address of 5917.

5957-6356 GAMMA* Not Applicable

6357-6596 DELTA Fixed boundary flux: Δ_{bg}

These are the boundary fixed source fluxes which are input for each boundary for each group.

6357 - right boundary flux, Group No. 1
6358 - left boundary flux, Group No. 1
6369 - right boundary flux, Group No. 2
6370 - left boundary flux, Group No. 2
. .
. .
. .
6585 - right boundary flux, Group No. 20
6586 - left boundary flux, Group No. 20

Address	Name	Description
6607-9186	SVM	Fixed volume source by point and group. Two values of SVM$_{ig}$ are required at each internal region boundary. The left and right problem boundaries require only one value. The addresses of these data must include the double value at each internal boundary. These values are the fixed volume sources for each group. The units on this source should be neutrons or photon energy per unit volume per unit time. The source values for q_{ig} for point i and group g are assumed to be isotropic.
9187-9315	POWR1	Fission density guess: This is fission density at each point. If NOT is input with a negative sign then POWR1 is punched as TAPAT problem output data on cards with addresses and these cards may be used as input guess for succeeding problem.
9316-9327	EMU*	Not applicable
9328-9407	CONC	Mixture atom densities, volume fractions, or physical densities for cross section mixing operations (NMIX values). (See NMIX and MIX in fixed point input and Section 3.5 for details.)
9408-11407	SC	Scalar Flux: N_{ig}. The scalar flux input, N_{ig}, is not a required input to TAPAT. The user may input fluxes from a previous problem to accelerate convergence of problems which include upscatter. The direct solution of fluxes in TAPAT from the source (i.e., a fission density or fixed source) does not require input fluxes except in upscatter problems. If NOT is input with a negative sign, then SC is punched as TAPAT problem output data as cards with addresses.
11408	SEN	Desired eigenvalue in search (zone thickness or concentration) problems. This quantity is initially set to 1.0 unless a value is input.
11409	RR	Concentration search parameter to allow variation of filler mixture with search mixture. The concentration search operation follows as: CONC(NFOS) = CONC(NFOS) + [RR * CONC(NSOS)]

Address	Name	Description
11410	EPS3	Convergence criterion on the search variable, CONC or DELR, for search calculations on concentration or zone thickness.
11411	BUCK	Transverse buckling specifications: The values of buckling (B^2) are input according to the options specified by the input value of N. If N = 0; one value of B^2 is entered as BUCK2(1). If N = 1; NGR values of B^2 are entered by group as BUCK2(1) to BUCK2(NGR) If N = 2; JMAX values of B^2 are entered as BUCK2(1) to BUCK2(JMAX).
12041-12640	DIFE	Diffusion coefficient (D_g) by group and mixture: The diffusion coefficient is either input as DIFE or calculated according to the input quantity MUTEST. If D_g's are to be calculated, the mixture numbers, MIR_m, must appear in ^{g} mixture operation (specified by NMIX, MIX, CONC) as a mixture of one or more constituents.

3.3 PROGRAM MISPHT, MIST, OR TOPIC (TRANSPORT THEORY) INPUT DATA

The following table is a description of the input quantities pertaining to the transport theory program (MISPHT, MIST or TOPIC) in the TAPAT system. These programs are selected if a 1, 2, or 3 are punched on the control card. The fixed and floating point data are entered under standard TAPAT formats described in Section 3.1.3.

3.3.1 Fixed Point Data

Address	Name	Description
1	MAX	Total number of mesh points (number of intervals plus one) $3 \leq MAX \leq 100$
2	JMAX	Total number of regions $1 \leq JMAX \leq 30$ A TAPAT region is a set of consecutive mesh intervals with the same ΔX or ΔR, and same mixture cross section set. Hence, if a variable mesh is desired in a single physical region, more than one TAPAT region must be used to describe a physical region.

Address	Name	Description
3	NGR	Total number of energy groups. $1 \leq NGR \leq 20$
4	NDS	Number of downscatter groups. $0 \leq NDS \leq 6$ The number of downscatter groups can be defined as one plus the maximum number of groups which can be skipped in scattering down from any group. It ranges from zero (no downscatter) to a maximum of 6 in TAPAT (e.g., Group 1 particles can scatter to Group 7).
5	NPS	Number of upscatter groups. $0 \leq NPS \leq 5$ The number of upscatter groups can be defined as one plus the maximum number of groups which can be skipped in scattering up from any group. It ranges from zero (no upscatter) to a maximum of 5 in TAPAT (e.g., Group NGR particles can scatter to Group NGR-5).
6	NOT*	Output control word. If NOT has a negative sign, the program punches fission density and group fluxes as TAPAT addressed decimal data cards and if the punched data are desired for each problem of a set of TAPAT problems, NOT must be a negative number for each problem. NOT = 0 - print eigenvalue, scalar fluxes, fission density NOT = 1 - print above information plus balance characteristics NOT = 2 - print above information plus angular fluxes (TOPIC average angular fluxes in the angle, ϕ.) NOT = 3 - TOPIC ONLY: print items (0, 1, 2) plus angular fluxes at the Gauss quadrature points in the angular direction, μ, ($\mu = \cos\theta$).
7	IG*	TOPIC ONLY: Number of inner iterations desired for angular flux calculations in the azimuthal angle, ϕ. This quantity has no effect in MIST or MISPHT. If there is NO anistropic scatter (all $\Sigma^{S_l}_{g \rightarrow g'} \equiv 0.0$) then IG should be set to 1. For all other problems IG = 3 or 4 is recommended.

* Input words with an asterisk are not the same in the diffusion theory codes. All other words are identical in both the diffusion and transport theory codes.

Address	Name	Description
8	ITOUT	Number of outer iterations; ITOUT = 0 specifies a single outer iteration, except in TOPIC where ITOUT = 3 or 4 which is required to converge angular fluxes. Maximum number of outer iterations is set at 50 unless otherwise specified. For a fixed distributed or boundary source problem, iterations are required in MIST and MISPHT only when fissionable materials are present and iterated fission density is desired or in TOPIC, when angular flux convergence is desired. When NOT>0, then ITOUT + 1 outer iterations (as a maximum) are done to store extra data needed for output edits.
9	LCO	Fission density convergence option. LCO = 0 - pointwise fission density convergence. LCO = 1 - eigenvalue (or total iterated fission density in a fixed source calculation) convergence.
10	NMIX	Number of pieces of data in the mixture vector.** (Equal to length of MIX or CONC vector.) If NMIX is negative, then a transverse leakage approximation correction (buckling) is applied to the cross sections. The buckling correction is applied to the cross section only if a mixture vector is used. $0 \leq NMIX \leq 80$ See explanation of the input data MIX and CONC as well as Section 3.5 for details.
11	MMIX	Number of cross section sets (elements, isotopes, or materials) to be read from the master cross section tape. This master tape is mounted on the MSFC IBSYS Version 13 Unit B-6. $0 \leq MMIX \leq 20$
12	MUTEST*	Angular interval option: There are three options for specifying angular intervals in the cos θ (Slab or Sphere) or cos ϕ (TOPIC) angular segmentation of the S_n approximation. MUTEST = 1: equal interval in cos θ (i.e., μ) or cos ϕ. MUTEST = 2: equal intervals in θ or ϕ. MUTEST = 3: input angular intervals with the values of EMU are input as floating point data for μ, or cos ϕ.

* Input words with an asterisk are not the same in the diffusion theory codes. All other words are identical in both the diffusion and transport theory codes.

** Note: The word vector is commonly used to describe a list of data.

Address	Name	Description
13	IDP	Input data print option. IDP = 0 - print input data IDP = 1 - do not print input data
14	JSP	Search calculation option. JSP = 0 - no search calculation, but perform an eigenvalue, distributed fixed source, or boundary fixed source calculation. JSP = 1 - concentration search calculation. JSP = 2 - zone thickness search calculation.
15	LPG	Fission density input guess option. LPG = 0 - flat guess, normalized to the input floating point data value, FAC. LPG = 1 - input pointwise guess with the integral normalized to the value, FAC. LPG = 2 - fission density guess from previous TAPAT problem preceding this problem (data still in memory core storage). The integral normalized to value, FAC. This word has no meaning if there are no fissionable regions in a problem. In distributed or boundary fixed source problems with no fissions, the fission density guess is set equal to zero for all mesh points.
16-45	II	Upper right (boundary) mesh point number for each region. Each region must have at least one interval. The first left boundary of a TAPAT problem is mesh point Number 1. (Each TAPAT region has a constant ΔR (or ΔX) within the region.)
46-75	MIR	Mixture cross section set number of the macroscopic cross section data which is to be used in each region; data are entered for Region No. 1 to Region No. JMAX. Mixture numbers are in reference to the mixture formed in the MIX vector or addressed input macroscopic cross section data. Each region must have a mixture number specified. (See Section 3.5 for more details.)
76-155	MIX	Mixture material cross section set numbers to specify the cross section mixtures to be formed. Each element of the mixture vector is a mixture or material number. The respective concentration, which is a volume fraction or atom density, is entered in the CONC vector (floating point data). Mixture number is given first and the constituent material numbers follow. In the CONC vector, a mixture number is designated.

Address	Name	Description
156	N*	Order of angular quadrature: This is the number of angular intervals in the cos θ or φ angular segmentation in the S_n approximation. N must be equal to 2 or 4 for S_2 or S_4 calculations. N is set equal to 4 if no value is input.
157	MIK*	Order of angular quadrature in the angle, θ, in TOPIC. This is the number of gauss quadrature points in μ halfspace as shown in Figure 4. A value of MIK up to and including 7 is allowed and MIK = 3 of 4 is recommended.
158-177	MTIX	Tape cross section set identification numbers to be read from the master tape. All identification numbers must appear in the same order in MTIX, as they appear on tape. Maximum number of sets is 20, and MTIXs are consistent with the tape.
178-197	NTMIX	Mixture or material set numbers corresponding to the tape set numbers (MTIX) to place tape cross section sets in Mixtures 1 - 30. The NTMIX set numbers permit the user to place a material or element cross section set from the master tape, designated by MTIX in the set number, NTMIX. Maximum number of sets is 20, and the value NTMIX must be less than or equal to 30. (See Section 3.5).
198	KREG	Region number, 1 through 30, to be used as the search zone thickness variable for the search option; JSP = 2.
199	NSOS	Position in mixture vector (1 through 80) of the material or mixture number and concentration to be the concentration search variable in the search option, JSP = 1. The value of NSOS specifies which material number, MIX, will be varied to achieve a desired eigenvalue. $2 \leq NSOS \leq NMIX$ and NSOS not equal to a position with CONC = 0.0.
200	NFOS	Position in mixture vector (1 through 80) of the material or mixture number and concentration to be the concentration search filler variable in the search option JSP = 1. NFOS = 0 allows no substitution of a material for changes in the concentration search variable (NSOS) material. $2 \leq NSOS \leq NMIX$ and $NFOS \neq NSOS$

* Input words with an asterisk are not the same in the diffusion theory codes. All other words are identical in both the diffusion and transport theory codes.

Address	Name	Description
201	KIT1	The number of outer iterations per search iterations. This allows the user to force new concentration or zone thicknesses search moves after each KIT1 outer iterations so that eigenvalue and search is converged simultaneously. $3 \leq KIT1 \leq 10$ and KIT1 = 3 or 4 recommended.
202	MFR*	Outer boundary mirror reflection option for TOPIC. This option allows the user to specify a correction to the outer boundary flux calculation of a cell calculation in TOPIC. MFR = 0, do not correct. MFR = 1, calculate correction at outer boundary.

3.3.2 Floating Point Data

1	EPS1*	Convergence criterion. EPS 1 has meaning only if there is fissionable material in the problem. EPS 1 is the convergence criterion on the pointwise fission density or integrated fission density. If LCO = 0: Pointwise convergence criteria of fission density must be met. If LCO = 1: Integral convergence criteria of fission density (eigenvalue) must be met. In using TOPIC for neutron or photon transport problems with fixed sources and no fission calculation, the value of EPS 1 is input as a negative number so that on the other iterations required to converge fluxes, no eigenvalue or fission density is calculated.
2	EPS2*	Group scalar flux convergence criterion. This criterion is used in TOPIC only. Successive mesh point scalar flux solutions must be within the criterion EPS 2. The value of EPS 2 must be greater than or equal to EPS 1 and a value of EPS 2 = 0.0 allows for eigenvalue or fission density convergence only as described for EPS 1.
3	XIN	The value of the radius or dimension at the center or left boundary. This word specifies the value of the slab dimension, cylinder radius, or sphere radius at the left (center or inner) boundary. It need not be zero, but it cannot be negative. $0.0 \leq XIN$

Address	Name	Description
4	THETA	Power extrapolation factor to be used to accelerate outer iteration convergence. A value of 0.0 or 0.2 is recommended to avoid excessive over-extrapolation. A value of $\theta = 0$ (or blank) corresponds to no extrapolation. A value of $\theta > 0.2$ can cause divergence of the fission density. The extrapolation procedure on the fission density guess for the next outer iteration N + 1 from the Nth and N-1 iterations as follows: $$P^{N+1} = P^{N}(1.0 - \theta) + P^{N-1}\theta$$
5	FAC	Fission density normalization factor. The total fission neutron source F_t which is calculated as: $$F_t = \sum_{g=1}^{NGR} \int_V \left(\nu_g \Sigma_g^f\right) N_g dV$$ is always used with FAC to obtain a value of the normalization parameter, FAC/F_t, and this value is used to multiply all fission density and flux values. FAC has no meanining in either a distributed or boundary fixed source problem. If no value for FAC is read in, it is automatically set equal to 1.0 by the program.
6	SGES	First guess of search variable modifier to be used in concentration or zone thickness search calculations. The value of SGES is the first modification of CONC or DELR, and the third and succeeding guesses are internally calculated by the program.
7-36	DELR	ΔR (or ΔX) specifications. The values of DELR are the interval widths ΔR (or ΔX) which are used in each TAPAT region. Each ΔR (or ΔX) must be greater than zero or an error indication will be printed.
37-636	SIGT	Total or transport cross sections by group and mixture**. This is the total collision (or transport corrected) cross section σ_g^t, entered by group and mixture. Either macroscopic or microscopic cross sections may be read in; but since only macroscopic values are used by the program, any microscopic cross section sets should be multiplied by the proper atom densities (by use of the cross section mixing operation

** A mixture cross section set is a macroscopic set of data which are used as a region material. Mixtures are composed of materials or elements, and may be input or internally calculated by the program.

Address	Name	Description

specified by NMIX, MIX, CONC). Cross sections for a given mixture can be read into the program without being used in any region of a given problem. This permits the user to read in all the cross section sets for a series of problems in the first TAPAT problem. Then one need only refer to the proper mixture numbers in the succeeding change cases:

37 - 56 Mixture 1, Groups 1 - 20
57 - 76 Mixture 2, Groups 1 - 20
. .
. .
. .
417 - 436 Mixture 20, Groups 1 - 20
. .
. .
. .
617 - 636 Mixture 30, Groups 1 - 20

Specific cross section address = 36 + [(Mixture No. -1)* (20)] + Group No. (See Table 1.)

637-1236 SIGS — Zeroth moment (P_o) scattering cross sections by group and mixture. This list of $\sigma^{S_0}_{g\rightarrow g}$ is, for each mixture, the cross sections for isotropic (zeroth moment) scattering within each group. These cross sections are only those for nondegrading scattering (no down-scatter). Cross sections are stored identical to SIGT with beginning address at 637. Specific cross-section address = 636 + [(Mixture No. - 1)* (20)] + Group No.

1237-1836 SIGS1 — First moment (P_1) scattering cross sections by group and mixture. This list of $\sigma^{S_1}_{g\rightarrow g}$ is, for each mixture, the cross sections for first moment non-degrading scattering (no down scatter) cross sections for scattering within each group. Cross sections are stored identical to SIGT with the beginning address at 1237. Specific cross section address = 1236 + [(Mixture No. - 1) * (20)] + Group No.

1837-2436 VUSIG — Neutron fission cross sections by group and mixture. The list of $\nu_g \sigma^f_g$ is, for each mixture, the neutron production cross sections (number of neutrons per fission times the fission cross section) for each group. Cross sections are stored identical to SIGT with beginning address of 1837. Specific cross-section address = 1836 + [(Mixture No. - 1) * (20)] + Group No.

Address	Name	Description
2437-2456	CHI	Fission neutron spectrum: χ_g: $\sum_{g=1}^{NGR} \chi_g \equiv 1.0$ for eigenvalue problems. The quantity, χ_g, defines the fraction of fission neutrons released in each group. For all problems at least one non-zero CHI must be input. The final eigenvalue in a TAPAT problem without fixed sources (distributed or boundary) is based on $\sum_{g=1}^{NGR} \chi_g$ neutrons in the system.
2457-5426	STR	Group to group transfer cross sections (downscatter) by mixture. This list of $\sigma^{S_0}_{g' \to g}$ values is for each mixture, the cross sections for isotropic (zeroth moment) transfer of neutrons or photon energy from each group to any of the lower energy groups. These cross sections govern the actual quantities of neutrons or photon energy which are transferred by down-scattering from one group to any other (maximum of six-group down scatter). This list is a truncated list of data containing only the possible non-zero entries. The entry of specific cross sections is illustrated in Table 1. Specific cross section address = 2456 + [(Mixture No. - 1) * 99] + Cross Section position from Table 1.
5427-5876	STRU	Group-to-group transfer cross sections (upscatter) by mixture. This list of $\sigma^{S_0}_{g \to g'}$ values gives for each mixture, the cross sections for isotropic (zeroth moment) transfer of neutrons from each group to any of the higher energy groups. These cross sections govern the actual quantities of neutrons which are transferred by upscattering from one group to any other group (maximum of five group upscatter). These transfers are limited to the bottom six groups of a TAPAT problem. This list is a truncated list of data containing only the possible non-zero entries. The entry of specific cross-section data is illustrated in Table 1. Specific cross section address = 5427 + [(Mixture No. - 1) * 15] + Cross Section position from Table 1.
5877-5916	ALPHA*	Boundary condition indicators: left and right boundary indicators for each group. These are the mirror albedo coefficients, a_{bg}. $ALPHA_{bg} = 0.0$: zero flux return condition, in which neutrons or photon energy crossing the boundary in group g are not reflected back across the boundary. $ALPHA_{bg} = 1.0$: mirror reflection or zero current condition in which all neutrons or photon energy are reflected back across the boundary in the "mirror image" of the angular directions.

Address	Name	Description
		ALPHA may assume any value such that $ALPHA_{bg}$ is the fraction of neutrons or photon energy reflected in the "mirror image" angular direction. 5877 left boundary, group No. 1 5878 right boundary, group No. 1 . . . . . . 5915 left boundary, group No. 20 5916 right boundary, group No. 20
5917-5956	BETA*	Isotropic albedo coefficients by boundary and group: These are the isotropic albedo coefficients, β_{bg}. For a given group, g, at a boundary b, the value of the coefficient β_{bg} is the fraction of all outbound particles which are reflected back in an isotropic (constant) angular distribution. Note: If the summation of plus $\alpha_{bg} + \beta_{bg}$ is greater than 1.0 at a boundary, there will be a multiplication of neutrons or photon energy (i.e., more neutrons or photon energy returned than leaving) at the boundary. $\beta_{bg} = 0.0$: no isotropic return of neutrons or photon energy. $\beta_{bg} > 0.0$: isotropic return of the fraction β_{bg} of neutrons or photon energy crossing the boundary. BETA's are input in a manner similar to the ALPHA's with an initial address of 5917.
5957-6356	GAMMA*	Polynominal coefficients: These are the boundary source coefficients which are given for each boundary for each group. They are the Legendre polynominal coefficients for a diffuse boundary source (as described in Section 2.2 and References 6, 7, 8) for $l = 0$ to 9 by boundary (left, right) and group number. These coefficients should be limited to $l \leq 1$ for TOPIC to eliminate errors in the boundary source.
6357-6596	DELTA*	Fixed boundary flux: These are the fixed boundary source fluxes, Δ_{bg} which are given for the relevant $\cos\theta$ or $\cos\phi$ quadrature points at each boundary for each group. For either a right or a left boundary (in a given group)

Address	Name	Description
		there must be $\frac{n}{2}$ + 1 values for the μ or cos φ solution points given. Hence for an S_4 case, three values of μ are required at either boundary for a group where one of the double values at μ = 0.0 in MIST; not required in MISPHT or TOPIC. 6357 - right flux μ = EMU (1) = 1.0, Group 1 6358 - right flux, μ = EMU (2) = μ_2 Group 1 6359 - right flux, μ = EMU (3) = 0.0, Group 1 6360 - left flux, μ = EMU (3) = 0.0, Group 1 6361 - left flux, μ = EMU (4) = μ_4 Group 1 6362 - left flux, μ = EMU (5) = 1.0, Group 1 6379 - right flux, μ = EMU (1) = 1.0, Group 2 6380 - right flux, μ = EMU (2) = μ_2 Group 2 6381 - right flux, μ = EMU (3) = 0.0, Group 2 . . . . . . etc. etc.
6607-9186	SVM	Fixed volume source by point and group. Two values of SVM_{ig} are required at each internal region boundary. The left and right problem boundaries require only one value. The addresses of these data must include the double value at each internal boundary. These values are the fixed volume sources for each group. The units on this source should be neutrons or photon energy per unit volume per unit time. The source values q_{ig} for point i and group g are assumed to be isotropic.
9187-9315	POWR1	Fission density guess: This is fission density at each point. If NOT is input with a negative sign then POWR1 is punched as output on cards with addresses.
9316-9327	EMU*	Angular interval option: These data are for the optional input specification of the points on the μ (μ = cos θ) halfspace for slab or sphere or for the cos φ halfspace in cylinders. Values of EMU are required only when MUTEST = 2.
9328-9407	CONC	Mixture atom densities, volume fractions, or physical densities for cross section mixing operations (NMIX values). (See NMIX and MIX in fixed point input and Section 3.5 for details.)

Address	Name	Description
9408-11407	SC	Scalar Flux: N_{ig} The scalar flux input, N_{ig}, is not a required input to TAPAT. The user may input fluxes from a previous problem to accelerate convergence of problems which include upscatter. The direct solution of fluxes in TAPAT from the source (i.e., a fission density or fixed source) does not require input fluxes except in upscatter problems.
11408	SEN	Desired eigenvalue in search (zone thickness or concentration) problems. This quantitiy is initially set to 1.0 unless a value is input.
11409	RR	Concentration search parameter to allow variation of filler mixture with search mixture. The concentration search operation follows as: CONC(NFOS) = CONC(NFOS) + RR * CONC(NSOS)
11410	EPS3	Convergence criterion on the search variable, CONC or DELR, for search calculations on concentration or zone thickness.
11411	BUCK*	Transverse buckling parameter specifications: These values are used in non-void regions to account for transverse leakage for the slab or cylindrical geometries BUCK (1) is X or X* for slab, or H or H* for cylinder. BUCK (2) is Y or Y* for slab. BUCK (3) is π (i.e. 3.14159) or 2.405 for calculations of group dependent buckling. BUCK (4) is 1.4209 for calculation of group dependent, extrapolation distance d, where d is the transport relaxation length $1.0/\Sigma_{tg}$ (i.e. λ_t) times the constant BUCK (4). (See Section 2.2.7 for details.)

3.4 DATA PROCESSING ROUTINES - INPUT DATA

Input requirements to the FLUX EDIT subprogram of the TAPAT system are dependent upon the type of operation to be performed. There are four distinct operations in FLUX EDIT. These are:

1) A fixed distributed source calculation routine based on separable spatial and energy distributions.

TABLE 1

TAPAT TRANSFER CROSS SECTION MATRICES

Downscatter Matrix

Position No.	Down 1	Down 2	Down 3	Down 4	Down 5	Down 6
1	$\sigma_{1\rightarrow2}$	20 $\sigma_{1\rightarrow3}$	38 $\sigma_{1\rightarrow4}$	55 $\sigma_{1\rightarrow5}$	71 $\sigma_{1\rightarrow6}$	86 $\sigma_{1\rightarrow7}$
2	$\sigma_{2\rightarrow3}$	21 $\sigma_{2\rightarrow4}$	. .	. .	. .	. .
3	$\sigma_{3\rightarrow4}$	.	. .	. .	. .	99 $\sigma_{14\rightarrow20}$
.	.	.	. .	. .	85 $\sigma_{15\rightarrow20}$	
.	.	.	. .	70 $\sigma_{16\rightarrow20}$		
.	.	.	54 $\sigma_{17\rightarrow20}$			
.	.	37 $\sigma_{18\rightarrow20}$				
19	$\sigma_{19\rightarrow20}$					

Specific material cross section address = 2466 +[(Material No. -1) * 99]+ Position No. in Table

TABLE 1 (CONTINUED)

Upscatter Matrix

Position No.	Up 1	Up 2	Up 3	Up 4	Up 5
1	$^{\sigma}$NGR→NGR-1	6$^{\sigma}$NGR→NGR-2	10$^{\sigma}$NGR→NGR-3	13$^{\sigma}$NGR→NGR-4	15$^{\sigma}$NGR→NGR-5
2	$^{\sigma}$NGR-1→NGR-2	.	.	14$^{\sigma}$NGR-1→NGR-5	
3	.	.	12$^{\sigma}$NGR-2→NGR-5		
4	.	9$^{\sigma}$NGR-3→NGR-5			
5	$^{\sigma}$NGR-4→NGR-5				

Specific material cross section address = 5427 + [(Material No. -1) * 15]+ Position No. in Table

2) A flux edit routine to calculate response functions (such as heating rates, dose rates, etc.) or distributed fixed source based on pointwise energy dependent flux data.

3) A program pause (PAUSE 7777) to allow tape handling between TAPAT problems.

4) A punch routine to output response function or photon source data on punched cards for subsequent input or plotting.

3.4.1 Fixed Distributed Source Routine

This routine generates a fixed distributed source (SVM_{ig}) in the TAPAT system from the separable spatial and energy distributions of a source. The user inputs a multigroup spectrum and a radial or axial pointwise distribution. This routine calculates the fixed distributed source for TAPAT and stores it properly in appropriate TAPAT addresses.

The input format for this routine is not the standard TAPAT format. A set of data is required to describe each region containing a source. The cards required for each region are described in the following table:

Card Type	FORTRAN Format	Name	Identification, Limits, Explanatory Notes
1	5I4	NG	Total number of groups in the distributed fixed source. $1 \leq NG \leq 20$
		NST	Mesh point number at left or inner boundary of the region containing this fixed source.
		MA	Mesh point number at right or outer boundary of the region containing this fixed source.
		JM	Region number containing this fixed distribution source.
		JLAST	A dual purpose control word to control: 1) print/punch of fixed distributed source; and 2) reading of new region source data or a following TAPAT problem. The following table indicates the function of JLAST.

	JLAST = 1	JLAST = 2	JLAST = 3	JLAST = 4
Print and Punch Fixed Source Data?	No	Yes	No	Yes
Last Region Data?	No	No	Yes	Yes

3.4.2 Flux Edit Routine

The flux edit routine calculates a response function or fixed distributed source based on pointwise flux data which was calculated in a previous TAPAT program or which is input by the user. This routine requires the same input data cards as TAPAT (program control - data type 1, title - data type 2, fixed point - data type 3, and floating point - data type 4), and uses the standard TAPAT input formats (see Section 3.1) except for the title card - data type 2. The flux edit title card is used to input control words as well as to input a title. The data required on a Flux Edit title card is described in the following table:

Card Type	FORTRAN Format	FORTRAN Symbol	Identification, Limits, Explanatory Notes
2	3I3, 10A6	IG1	Geometry function control word to be used for integration and normalization of data in the flux edit routine. IG1 = 0, Slab geometry calculation. IG1 = 1, Cylindrical geometry calculation. IG1 = 2, Spherical geometry calculation.
		IG3	Program control word for data input, source initialization, and source accumulation (See Table 2).
		NGG	Number of groups in the distributed fixed source (e.g., 13 photon energy groups).
		TITLE	Any 60 character alphanumeric title

TABLE 2

IG3 CONTROL OPTIONS IN FLUX EDIT

Operation	IG3 = -1, -2, -3, or -4	IG3 = 0	IG3 = 1	IG3 = 2	IG3 = 3	IG3 = 4
Read Input Data (Fixed and Floating Point Data)	Yes	No	Yes	Yes	Yes	No
Initialize Distributed Fixed Source Storage Locations (Set $SVM_i^g = 0.0$)	No	No	No	Yes	No	No
Calculate Response or Reaction Rate	Yes	Yes	Yes	Yes	Yes	No
Accumulate Distributed Fixed Source, SVM_i^g over Materials and Reactions	Yes except for a -1	No	No	Yes	Yes	No
Integrate Response Function or Reaction Rate Data	Yes	Yes	Yes	Yes	Yes	No
Integrate Distributed Fixed Source Data	No	No	No	No	No	Yes

The manner in which the fixed and floating point input data are used by the FLUX EDIT program is described in Section 2.4. It is important to note that the fixed and floating point data must either be input by the user or must be present in core memory from a previous TAPAT program. The POINT Program (Volume 2) prepares an input deck for FLUX EDIT which contains all data required for energy deposition or for distributed fixed source calculations. However, the standard problem input data of (MAX, JMAX, NGR, II, MIR, DELR, and XIM), and the flux data must be present in core memory storage or must be input as the POINT program output data. If specialized calculations are desired from FLUX EDIT, the user must input special response function data (e.g. dose rate). The types of fixed and floating point input data required to run the FLUX EDIT routine are described as follows:

Fixed Point Data

Address	Name	Identification
1	MAX	Total number of mesh points (Number of intervals plus one) $3 \leq MAX \leq 100$
2	JMAX	Total number of regions $1 \leq JMAX \leq 30$
3	NGR	Total number of energy groups $1 \leq NGR \leq 20$
16-45	II	Upper (right boundary) mesh point number for each region. Each region must have at least one interval. The first left boundary is point number 1.
46-75	MIR	Material number of the material which is used in each region; from region No. 1 to JMAX. Material numbers are in reference to the MIX vector or addressed input cross section data. Each region must have a material number specified. (See Section 3.5 for details.)

Floating Point Data

Address	Name	Identification
3	XIN	The value of the radius or dimension at the center or left boundary. This word specifies the value of the slab dimension, cylinder radius, or sphere radius at the left (center or inner) boundary. It need not be zero, but it cannot be negative. $0.0 \leq XIN$
7-36	DELR	ΔR (or ΔX) specifications. The values of DELR are the interval widths ΔR (or ΔX) which are used in each TAPAT region. Each ΔR (or ΔX) must be greater than zero or an error indication will be printed.
1837-2436	VUSIG	Reaction cross sections (or response function values) for each group, g, and each material, m, corresponds to the MIR input. NOTE: This quantity allows the user to calculate a variety of data, such as dose rates, heating rates, sources, etc., by inputting the proper quantity at $VUSIG_{gm}$.
2437-2456	CHI	Energy or particle distribution by group, g.

3.4.3 Pause Routine

This option is included to permit a cross section tape change (neutron to photon) and is not a recommended operation. If cross section tape input is to be used, then the user may best use TAPAT by using a combined (neutron and photon) master cross section tape. The POINT program (Volume 2) prepares a TAPAT macroscopic cross section deck for neutrons and photon transport; hence, this option is not required when the POINT Program cross section data are used.

3.4.4 Punch Routine

This routine is a punch routine to obtain mesh point coordinates and reaction rate or response function data calculated by the FLUX EDIT routine. This data is punched in

FORTRAN Format 6E12.5. The three sets of data punched are: (1) flux mesh point coordinates, (2) the reaction or response rate data at each mesh point including two values at each internal region boundary, and (3) the source mesh point coordinates with two values at each internal mesh.

3.5 DETAILED DESCRIPTION OF SELECTED INPUT DATA

3.5.1 Example of Material Input Data

One of the useful features of the TAPAT system is the variety of ways in which cross section and material data can be input to the code. Because there are so many ways of inputting the data, it is difficult in the input data sections (Sections 3.2 and 3.3) to describe precisely how these data can be setup.

Two examples are given here to clarify that section of the input data:

Example 1

Region No.	Description
1	Hydrogen gas
2	Steel
3	Water
4	Water (50% by vol.) Steel (50% by vol.)
5	Uranium (50% by vol.) Water (50% by vol.)
6	Void (no material)
7	Steel

If microscopic cross section data for various elements are on a tape, then the following elements must be called from tape to describe the materials in the problem:

hydrogen, oxygen, iron, nickel, chrome, and uranium. These elements must be obtained from the tape by ascending number as follows:

MTIX (Tape Element No.)	Element
25	Hyd
27	Oxy
30	Fe
33	Ni
51	Cr
67	U

Next, the tape element numbers (MTIX) are assigned NTMIX numbers by the user (see Sections 3.2 and 3.3) as follows:

MTIX (Tape Element No.)	NTMIX	Element
25	1	Hyd
27	2	Oxy
30	3	Fe
33	4	Ni
51	5	Cr
67	6	U

The program now assigns the NTMIX No. 1 to the hydrogen data, No. 2 to the oxygen data, etc.

Next, the user should assign an MIR number to each region (see Section 3.2 and 3.3) as follows:

Region No.	Description	MIR No.
1	Hydrogen gas	7
2	Steel	8
3	Water	9
4	Water (50% by vol.) Steel (50% by vol.)	10
5	Uranium (50% by vol.) Water (50% by vol.)	11
6	Void (no material)	12
7	Steel	8

The user should next mix the NTMIX numbers into the MIR Region number to form the MIX data, and set up his CONC vector at the same time as follows:

(Floating Point) CONC Vector	(Fixed Point) MIX Vector
0.0	7 (MIR No.)
Hyd atom density	1 (MTMIX No.)
0.0	8 (MIR No.)
Fe atom density	3 (NTMIX No.)
Ni atom density	4 (NTMIX No.)
Cr atom density	5 (NTMIX No.)
0.0	9 (MIR No.)
Hyd atom density	1 (NTMIX No.)
Oxy atom density	2 (NTMIX No.)
0.0	10 (MIR No.)
0.5 (water vol. fraction)	9 (MIR No.)
0.5 (steel vol. fraction)	8 (MIR No.)
0.0	11 (MIR No.)
Uranium atom density	6 (NTMIX No.)
0.5 (water vol. fraction)	9 (MIR No.)
0.0	12 MIR No. (If memory is not cleared
1.0 E-10	2 NTMIX No. at beginning of problem)

Several items in the above table should be noted: (1) atom densities and volume fractions can be used in the CONC vectors for a region if the region contains a material previously described by an MIR No. (such as water in the example); (2) a CONC value of 0.0 must be associated with each MIR No. of a region to denote composition change, and, (3) no cross section data are employed for a "void" since it is assigned an MIR No. of 12 which contains all "zeros" (if memory was cleared by inserting the 99 on the problem title card).

Example 2

Consider a problem having the following three regions:

Region No.	Description
1	Uranium (50% by vol.) Carbon (50% by vol.)
2	Water
3	Steel

If macroscopic cross section data for each region are on tape, the following table should be set up:

MTIX (Tape No.)	Region No.
38	1
46	2
47	3

Next, the tape element numbers (MTIX) are assigned NTMIX numbers by the user as follows:

MTIX (Tape No.)	NTMIX
38	1
46	2
47	3

The user should assign an MIR number to each region as follows:

MIR No.	Region No.
6	1
7	2
8	3

The MIX and CONC vectors are simply input as follows:

(Floating Point) CONC Vector	(Fixed Point) MIX Vector
0.0	6 (MIR No.)
1.0	1 (NTMIX No.)
0.0	7 (MIR No.)
1.0	2 (NTMIX No.)
0.0	8 (MIR No.)
1.0	3 (NTMIX No.)

3.5.2 Determination of Mesh Interval Size

In order to define the mesh point interval size in TAPAT neutron or photon transport problems, a few simple rules are presented here. If the TAPAT mesh point limitation of 100 mesh points does not allow the program user to follow these guidelines, the techniques to define the minimum necessary mesh coordinate dimensions are illustrated.

The experience obtained in using TAPAT has resulted in the use of the empirical relationships as suggested by Putnam.[6,7] These criteria which are based on angular quadrature and region total and scattering cross sections, are considered to be "safe" criteria. The empirical relationships are stringent and considerable intuitive judgment is required in applying these criteria.

The radial mesh interval size in a TOPIC calculation is approximated by the following equation:

Criteria 1:

$$\Delta R = \frac{1.0 + \left[\Sigma^{S_0}_{g \to g} \Big/ \Sigma^{t}_{g} \right]}{\Sigma^{t}_{g} \quad (N-1)}$$

where:

N = the order of angular quadrature (e.g., S_4 calculation, $N = 4$)

Σ^{t}_{g} = the largest total (transport corrected) group cross section in the region

$\Sigma^{S_0}_{g \to g}$ = the corresponding within group scattering cross section in the region.

The mesh interval size in a MIST calculation is approximated by the following equation:

Criteria 2:

$$\Delta X = {}^{2.0}\Big/_{\Sigma^{t}_{g}}$$

where:

Σ^{t}_{g} = the largest total (transport corrected) group cross section in the region.

In problems where the limitation of 100 mesh points prevents adherence to the above two guidelines, an intuitive choice of mesh must be made to avoid questionable results. The following procedure should be followed:

Criteria 3: Criteria 1 and 2 should be applied near region boundaries where large flux gradients occur.

Criteria 4: Mesh size should not vary more than a factor of two between adjacent mesh intervals (i.e., criteria 1 and 2 can be relaxed within a region).

Criteria 5: The intervals near the periphery of a reflected core in all problems should follow criteria 1 and 2.

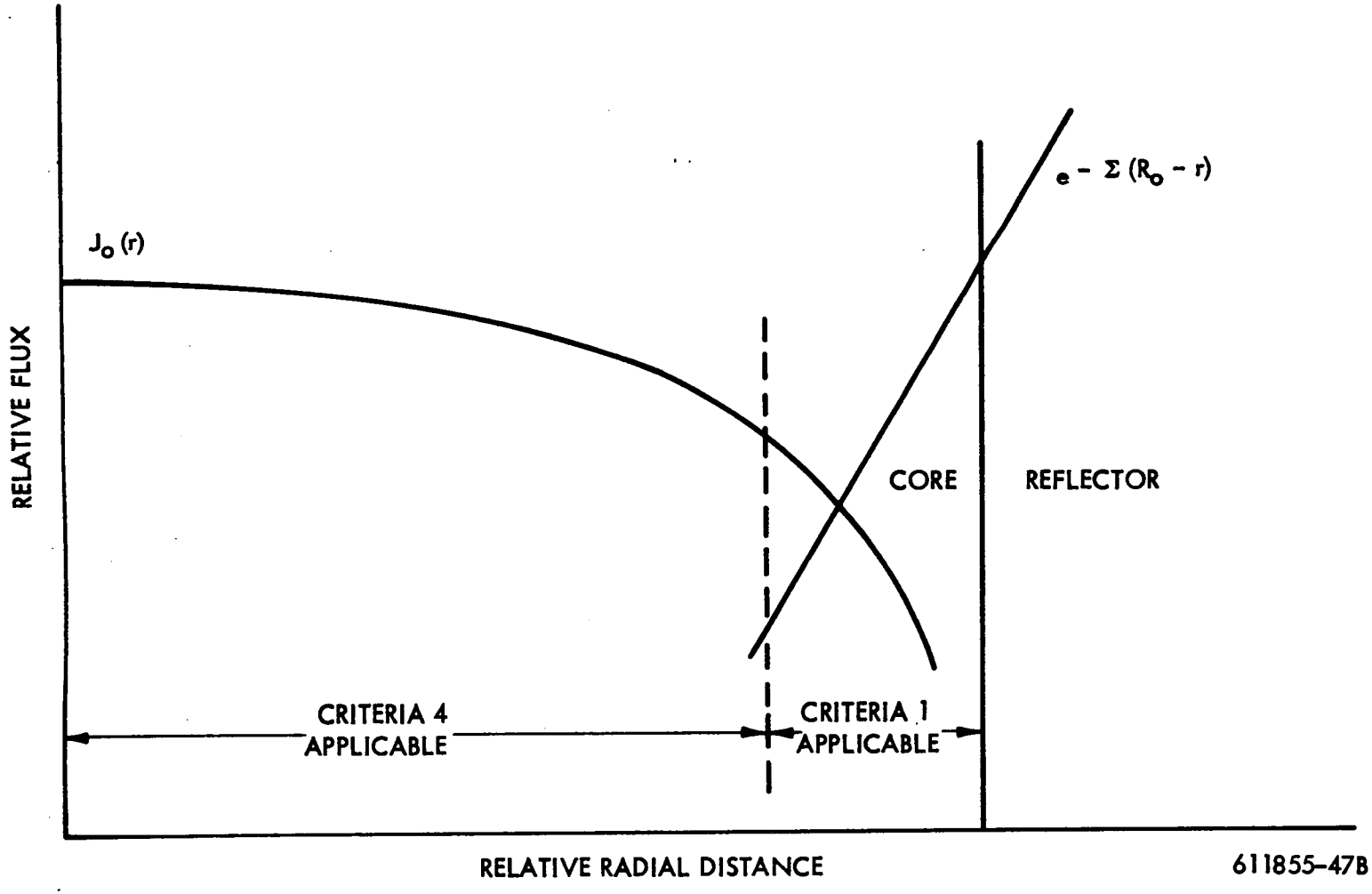
The remainder of the radial mesh in the core, reflector, etc., can be determined by criteria 4. (See Figure 7 for clarification.)

Justification for usage of criteria 3, 4, and 5 is based on the knowledge that most of the neutron or photon energy at any point in a region is produced by sources or scattering down from higher groups rather than direct transport from neighboring points. At the periphery of a reflected reactor, this condition does not exist because of the returning thermal neutrons from the reflector; hence, criteria 1 should be applied at the periphery of the core if negative fluxes are to be avoided.

Although negative fluxes may occur using criteria 3, 4, and 5, the location of these negative fluxes and the relative flux level surrounding the negative flux should now have a negligible effect on the overall problem solution.

In the TAPAT transport program, an approximation of mesh interval size in large non-central void regions (such as the void between a reactor and an external shield) may be represented by a method suggested by Putnam:

"... solutions in non-central voids may be possible by choosing mesh intervals in the void region as if a total cross section of $\Sigma_g^t = 1/\bar{r}$ existed in the region (where $\bar{r}$ is a mean radius). If a large expanse of noncentral void exists, it saves on mesh lines to define several contiguous void regions with different r mesh interval sizes to permit fewer mesh intervals in the outer regions where $\bar{r}$ is larger."



NOTE: THE JUNCTION OF CRITERIA 1 AND 4 OCCURS AT THE POSITION WHERE THE REFLECTOR NEUTRONS IN A GROUP CONTRIBUTE A NEGLIGIBLE AMOUNT TO THE TOTAL FLUX IN THAT GROUP.

Figure 7. Graphical Interpolation of Minimum Mesh Line Requirements in a TAPAT Problem

Neutron transport calculations using TAPAT have been performed using the recommendations outlined above and the creditability of the determination of mesh interval sizing has been proven in practice.

3.6 EXPLANATION OF INPUT ERROR INDICATORS

When an input data error is detected by the TAPAT program system, an error indication is printed off-line, and the problem is terminated.

In the following list, the underlined words are the error indication statements which are printed off-line. The explanation of the error then follows.

1. Error, Address Format for Fixed Point Data
   a) Number of data words on card (Cols. 1-2) is zero, negative, or greater than twenty-one (21).
   b) Fixed point address (Cols. 4-7) is zero, negative, or greater than 202.
2. Error, Address Format for Floating Point Data
   a) Number of data words on card (Cols. 1-2) is zero, negative, or greater than 6.
   b) Floating point address (Cols. 4-7) is zero, negative, or greater than 11410 (12641 for the ADDICT subprogram).
3. Error, Number of Points too Large

   The number of mesh points I = MAX, has been set to greater than 100.
4. Error, Number of Points too Small

   I = MAX has been set too small, i.e., less than three.
5. Error, Number of Regions Too Large

   JMAX has been set greater than thirty.
6. Error, Number of Regions is Zero

   JMAX has been set ≤ 0.
7. Error, Number of Groups too Large

   NGR has been set greater than twenty.

8. Error, Number of Groups is Zero

   NGR has been set ≤ 0.

9. Error, Number of Downscatter Groups too Large

   NDS has been set greater than 6.

10. Error, Number of Upscatter Groups too Large

    NPS has been set greater than 5.

11. Error, Zero or Negative Material Number

    A material number, MIR, for some region has been set ≤ 0, or has been left out.

12. Error, Material Number Greater than 30

    A material number, MIR, for some region has been set greater than thirty.

13. Error, Upper Region Boundary Non-Increasing or II(1) is Less than or Equal to 1

    Either II(J) is $\leq$ II(J-1) for some $1 \leq J \leq JMAX$; or II(1) ≤ 1; i.e., some region contains less than one mesh interval.

14. Error, Zero Delta R

    The interval width, DELR, has been set ≤ 0 for some region.

15. Mixing Vector Must Have at Least Two Elements

    NMIX has been set equal to 1. It must be at least two, if it is not zero.

16. Inconsistent Concentration Vector

    One or more of the following erroneous specifications have been made:

    a) CONC(1) $\neq 0$,

    b) Either CONC(NMIX) = 0 or NMIX is too large, or

    c) Two successive CONC values are zero.

17. Material Number Greater than 30 in Mixture Vector

    Some number in the MIX list is greater than thirty.

18. Error, Inconsistent Angular Input

    One or more of the following has occurred:

    a) N, the number of intervals on the μ or ϕ halfspace is too large for the sub-program being run.

    b) N, is an odd integer.

    c) angular interval specifications (EMU) are inconsistent.

19. Error, No Fission Cross Sections or Sources

There are no non-zero values for ν_g^f in any group for any region, and there are no fixed sources, either volume sources or boundary sources; therefore, no non-trivial solution exists. The MIR list may be wrong; i.e., a fissioning material may have been left off the list.

20. Error, No Non-Zero Chi

There are fissions (i.e., some non-zero ν_g^f in some group) in some region but χ_g, the fission spectrum, is zero for all groups.

21. Error, Zero Diffusion Coefficient

(ADDICT only)

There is a region mixture specified by MIR which has a zero diffusion coefficient; the MIR list or MIX list may not include consistent data.

SECTION

4.0 PROGRAM LOGIC

The TAPAT program system is a package of five subprograms written in FORTRAN IV and assembled with the IBM IBSYS Version 13 Monitor System. The entire system uses the overlay mode of FORTRAN IV and operates in the alternate input/output package (ALTIO) of the IBSYS monitor system. The first two subprograms of TAPAT (FLUX EDIT and ADDICT) are contained in the same overlay in order to reduce the number of overlays in the TAPAT program system. The sixteen subprograms of TAPAT allow the solution of up to a 100 mesh point diffusion or S_n transport approximation problem. The transport programs are limited to an S_4 or an S_2 angular approximation. The input format for each subprogram is the same except for the FLUX EDIT data processing subprogram.

A FORTRAN source deck listing of the TAPAT system is not presented in this report since there are approximately 12,000 FORTRAN statement cards in the system.

Because of memory core storage limitations, each subprogram is divided logically into 4 overlays. (The overlay feature of the IBSYS Monitor allows parts of a program to be stored on magnetic tape and to be subsequently called off the tape into memory core storage when needed. These overlays transfer data by means of labeled common storage.) The general logical function of the main TAPAT program and of each overlay, and each of the subroutines contained in each overlay is as follows:

The entire TAPAT system is controlled by a main program, which initializes (sets to 0.or 0.0) all labeled common storage data locations and calls the subprogram specified by the input control word (Data Type 1). The overlay level of each subprogram is the ALPHA level and each subprogram is subdivided into 4 overlays. This second level overlay is designated the BETA, GAMMA, SIGMA, and PI levels within each subprogram. The function of each subprogram and its overlay level follow as:

FIRST ALPHA OVERLAY

This overlay contains the FLUX EDIT subprogram and the ADDICT diffusion theory subprogram. The four overlays (level BETA) and their function follows as:

First BETA Overlay

This overlay contains the FLUX EDIT subprogram, and it is subdivided into four calculation routines which calculate reaction rate and/or distributed fixed source data and can provide printed and punched output of the calculated rate and other TAPAT problem results.

Second BETA Overlay

This overlay which is the first portion of the ADDICT subprogram, reads, checks and prints the input data; it calculates geometric data; mixes cross sections; calculates the fission source; and calculates search variable data.

Subroutines	
INPRX	prints input data
SCHECX	calculates the fission source
MIXXX	forms the cross section mixtures
SEARCHX	calculates the search variables

Third BETA Overlay

This overlay performs the solution for all the fluxes of each group in each outer iteration of the diffusion theory program, ADDICT. This overlay obtains the new fission source on each outer iteration, and checks for satisfaction of the convergence criteria.

Subroutines	
SOURCE	calculate the difference equation coefficients of each group.
FLUX	uses the coefficients from the SOURCE subroutine to backsolve and obtain fluxes for each group.
CONV	calculates a new fission source and checks it for satisfaction of the convergence criteria.

Fourth BETA Overlay

This chain performs the edits for almost all of the output. (See Section 5.0 Output Description).

SECOND ALPHA OVERLAY

This overlay contains the spherical (MISPHT) subprogram of TAPAT. The four overlays within MISPHT (overlay level GAMMA) and their function follow as:

First Gamma Overlay

This chain reads, checks and prints the input data; it initializes angular and geometric data; mixes cross sections; calculates the fission source, and calculates search variable data.

Subroutine	
INPR	prints input data
SCHECK	initializes the fission source
MIXX	forms the cross section mixtures
SEARCH	calculates the search variables

Second Gamma Overlay

This chain computes the matrix coefficients for each group, computes the elements of each matrix to be used in the solution, and stores those matrix elements on duplicate binary tapes.

Subroutines	
OPINT, SETUP, ALQS, AQSJL	Calculates auxiliary coefficients for use in computing the elements of the original matrix for each group.
BUNDRY	Calculates the matrix elements and source vector elements for each group which depend on the boundary condition equations.
MTXSET	Calculates the matrix elements for each group which depend on the basic balance equation.
FACTOR	operates on the matrix elements calculated in MTXSET to produce the matrices to be used in the solution of angular fluxes.

Third Gamma Overlay

This chain obtains the solution for all the fluxes of each group in each outer iteration of the MISPHT subprogram. This overlay also obtains the new fission source on each outer iteration, and checks for satisfaction of the convergence criteria.

Subroutines	
SOURCE	multiplies the source vector of each group by one of the solution matrices.
FLUX	uses the second matrix and the result from the SOURCE subroutine to backsolve and obtain angular fluxes for each group.
CONV	calculates a new fission source and checks it for satisfaction of the convergence criteria;

Fourth Gamma Overlay

This chain performs the edits for almost all of the output. (See Section 5.0 Output Description.)

THIRD ALPHA OVERLAY

This overlay contains the spherical (MIST) subprogram of TAPAT. The four overlays within MIST (overlay level SIGMA) and their function follow as:

First SIGMA Overlay

This chain reads, checks and prints the input data; it initializes angular and geometric data; mixes cross sections; calculates the fission source, and calculates search variable data.

Subroutine	
INPR	prints input data
SCHECK	initializes the fission source
MIXX	forms the cross section mixtures
SEARCH	calculates the search variables

Second SIGMA Overlay

This chain computes the matrix coefficients for each group, computes the elements of each matrix to be used in the solution, and stores those matrix elements on duplicate binary tapes.

Subroutines

OPINT, SETUP, ALQS, AQSJL	calculates auxiliary coefficients for use in computing the elements of the original matrix for each group.
BUNDRY	calculates the matrix elements and source vector elements for each group which depend on the boundary condition equations.
MTXSET	calculates the matrix elements for each group which depend on the basic balance equation.
FACTOR	operates on the matrix elements calculated in MTXSET to produce the matrices to be used in the solution of angular fluxes.

Third SIGMA Overlay

This chain obtains the solution for all the fluxes of each group in each outer iteration of the MIST subprogram. This overlay also obtains the new fission source on each outer iteration, and checks for satisfaction of the convergence criteria.

Subroutines

SOURCE	multiplies the source vector of each group by one of the solution matrices.
FLUX	uses the second matrix and the result from the SOURCE subroutine to backsolve and obtain angular fluxes for each group.
CONV	calculates a new fission source and checks it for satisfaction of the convergence criteria.

Fourth SIGMA Overlay

This chain performs the edits for nearly all of the output. (See Section 5.0 Output Description.)

FOURTH ALPHA OVERLAY

This overlay contains the cylindrical geometry (TOPIC) subprogram of TAPAT. The four overlays with TOPIC (overlay levels PI) and their function follow as:

First PI Overlay

This overlay reads, checks and prints the input data; it initalizes angular and geometric data; mixes cross sections; calculates (i.e. initializes the fission source) and computes search variable data.

Subroutines

INPRX	prints input data
SCHECX	initializes the fission source
MIXXX	forms the cross section mixtures
SEARCX	calculates the search variables

Second PI Overlay

This chain computes the matrix coefficients for each group; computes the elements of each matrix to be used in the solution of the matrix and stores those matrices on duplicate binary tapes.

Subroutines

SSET	calculates various data needed for the Gauss quadrature
BUNDRY	calculates the matrix elements and source vector for each group which depend on the boundary condition equations.
MTXSET	calculates the matrix elements for each group which depend on the basic balance equation.

Subroutines

MTXSEL	calculates and stores on tape the intermediate coefficients which are used to solve for the Gauss quadrature point fluxes for points greater than 1 in each group.
FACTOR	operates on the matrix elements calculated in MTXSET to produce the matrices to be used in the solution of angular fluxes.

Third PI Overlay

This chain obtains the solution for all the fluxes of each group in each outer iteration of the TOPIC subprogram. This overlay also obtains the new fission sources on each outer iteration, and checks for satisfaction of the convergence criteria.

Subroutines

SOURCE	multiplies the source vector of each group by one of the solution matrices.
FLUX	uses the second solution matrix and the result from the SOURCE subroutine to backsolve and obtain angular fluxes for each group.
HIMODE	uses angular fluxes obtained in the FLUX subroutine to obtain Gauss quadrature angular fluxes for Guass points greater than 1.
CONV	calculates a new fission source and checks it for satisfaction of the convergence criteria.

Fourth PI Overlay

This chain performs the edits for almost all of the output. (See Section 5.0 Output Description.)

TAPE ASSIGNMENTS

The logical tape assignments as explicitly used in the FORTRAN input-output statements are:

	Logical	MSFC IBSYS Version 13 Tape
All BCD output	Tape 6	B - 1
All BCD input	Tape 5	A - 3
All BCD punch output	Tape 7	B - 2
Intermediate binary	Tape 2	B - 3
Intermediate binary	Tape 4	B - 4
Intermediate binary	Tape 8	A - 5
Intermediate binary	Tape 9	B - 5
Intermediate binary	Tape 10	A - 6
Master Cross Section tape	Tape 11	B - 6

In addition, the overlays are stacked on logical Tape 3.

SECTION

5.0 OUTPUT DATA DESCRIPTION

The amount of printed or punched output data obtained from a TAPAT problem is dependent on the subprogram being used and the input control words. The output is discussed specifically for the FLUX EDIT subprogram, and generally for the other TAPAT subprograms (ADDICT, MISPHT, MIST, TOPIC).

5.1 FLUX EDIT SUBPROGRAM

The printed and punched output from a FLUX EDIT problem is dependent upon the routine used in the FLUX EDIT subprogram. The three routines which provide printed or punched output data are the fixed source, flux edit and punch routines.

5.1.1 Fixed Source Generation Routine

The printed and punched output from the fixed source generation problem is controlled by the values of the input quantity, JLAST. The first printed line (if any) of each fixed source generation problem (a single region calculation) is the title line: FIXED SOURCE INPUT BY POINT AND GROUP. The next printed output is a printed line corresponding to each TAPAT input quantity and containing (a) the number of pieces of data on the card, (b) the address of the first piece of data on the card, and (c) the fixed source data as calculated in the routine. The set of TAPAT input cards for the single region or for a set of regions can be obtained as printed output by use of the input quantity, JLAST. The punched output data from the fixed source generation routine are the TAPAT cards corresponding to the printed data above.

5.1.2 Flux Edit Routine

The printed output from the flux edit routine is obtained for each reaction rate calculation. The first line of the printed output is the title information on the first card of each flux edit problem deck. The next line is obtained only for the final fixed source edit of the multigroup source data at each mesh point. This printed line is obtained for each group (and the titles that follow the data,) as FIXED SOURCE GROUP N, where N is the particular group. The next line of printed data is the title of each column of data to follow. Each

succeeding line contains the flux mesh point number, mesh point coordinate, mixture at the mesh point, reaction rate, normalized reaction rate, and at the first mesh point in each region, volume or area integrated reaction rate, and the average reaction rate in the region. Each set of region data is separated by a row of asterisks.

The printed neutron or photon source data are obtained under control of the input data quantity IG3. The photon source data is obtained as discussed above except that the fixed source data is obtained instead of reaction rate data.

5.2 OTHER TAPAT SUBPROGRAMS

The amount of output data normally obtained off-line from a given TAPAT problem is controlled by the two fixed point input words, NOT and IDP.

The first line of the output data always contains the data on the Alphanumeric card of the problem; the next line tells which subprogram of TAPAT is being run (ADDICT, MISPHT, MIST, or TOPIC).

5.2.1 The Input Data Edit

If IDP is less than 1, the next data listed consists of an edit of the problem input data. The input data listed are:

1) the fixed point data consisting of IG, MAX, JMAX, NGR, NDS, MUTEST, N, LPG, LCO, NOT, NMIX, IDP, ITOUT, MIK (TOPIC only), NPS, MMIX, JSP, KREG, NSOS, NFOS.
2) the floating point data consisting of EPS1, EPS2 (TOPIC only), XIN, THETA, FAC, SGES, SEN, RR.
3) the basic region data consisting of (for each region) the region number, the material used in the region, the upper r mesh point value of the region, the Δr of the region, and the upper value of r for the region (i.e., J, MIR(J), II(J), DELR(J), and the value of r_i for i = II(J).
4) the angular interval data consisting of the cos θ or cos ϕ_j value for each value of the index j on the μ or ϕ halfspace.
5) the cross section mixture data (if any) consisting of the values of CONC and MIX corresponding to each numbered position in the mixture vector.

6) the fixed volume source data (if any) consisting of the value of SVM at every source point for each group (There are MAX + JMAX-1 source points listed for each group.)

7) the boundary condition specification data for each group

8) the cross section data for each region consisting, first, of the values of σ_g^t, σ_g^{S0}, σ_g^{S1}, and σ_g, σ_g^f (ADDICT only: σ_g^t, σ_g^R, D_g, σ_g, σ_g^f, B_g^2) for each group and, second, of the values of the transfer or down and up scattering cross sections.

9) finally, the fission spectrum data consisting of the value of CHI (χ_g) for each group.

5.2.2 Outer Iteration Monitor

At the end of each outer iteration, a set of data is printed out which summarizes the rate and degree of convergence of various quantities. These data are in two sections:

The next lines of data give the fission source convergence summary. It consists of the iteration number (n), the eigenvalue λ_n in eigenvalue problems or the value of P_n in fixed source problems, E_{max} (EMAX), E_{min} (EMIN), the value of the convergence for LCO = 0 or 1 and the value of the input word EPS1.

For TOPIC only, the next G+1 (NGR $\leq$ 1) lines of data give the scalar flux convergence summary for each group. The iteration number n is printed first. This is followed by G lines which give, for each group, the following data: the group number g, the maximum value of the scalar flux ratio, the point i at which this maximum occurs, the minimum value of the scalar flux ratio, the point i at which this minimum occurs, the value of calculated convergence and the input word EPS2.

5.2.3 Problem Solution Output

The first line printed as output for the converged problem simply states the final outer iteration number, n, and either λ_n or P_n, depending on whether the problem is an eigenvalue or fixed source problem. If there are no fissions, this line is replaced by one which states "No Fission Problem--No Eigenvalue".

Next, MAX + JMAX-1 (the number of source mesh points) lines are printed. On each line there are listed: the mesh point index number i on r, the value of r_i, the material number MIR at the point, the fission source distribution $P_n(r_i)$ (Right and left hand values are given at each region interface for MIR and $P_n(r_i)$), and the value of the scalar flux $\phi(r_i)$ for each of the groups.

The data described above are always obtained. In addition, if NOT ≥ 2, the next data printed for each group are: For each mesh point r, there is printed the value of i, the value of r_i, the net current $J(r_i)$, the left hemispherical current $J(r_i)$, the right current $J(r_i)$, and the values of the average angular flux $N(r_i, \mu_i)$ or $N(r_i, \phi_i)$ for each quadrature point.

If NOT ≥ 1, the next data listed are the balance characteristics for each group. These data for each group consist of JMAX + 1 lines of data--one for each region and one for the total of all the regions. For each region there are listed: the region number, the integrated flux of the region, the integrated fixed volume source, the total absorptions (in TOPIC and MIST this data includes transverse leakage), the total fissions divided by λ_n, the net leakage, and for TOPIC only, the average flux, and the average fission source. These data are followed by a line of data giving the sum over all regions for each of the above quantities except for the average quantities. The average flux and average fission source values printed in TOPIC on the "Total" line for each group are only for regions with fissions.

For ADDICT only, the transverse leakage (T LEAKAGE) is obtained as the right column of printed data. When all these data for each group are listed, a line is printed which totals the stated quantities for all groups as well as all regions. In the case for TOPIC, the average flux and average fission source values printed are simply the sums of the values printed on the "Total" line for each group.

For ADDICT only, the groupwise balance table containing all the above quantities for regions is obtained.

In TOPIC only, if NOT=3, the last data output are the detailed angular flux values for each group. For each group and each Gauss point, there are listed for each flux mesh point the following data: the mesh point index i, the mesh coordinate value, and the values of angular flux for each flux solution point on a Gauss point.

SECTION

6.0 OPERATING INSTRUCTIONS

The operating instructions and card deck setup for TAPAT problems are similar to any FORTRAN IV production problem to be run with the IBM IBSYS Version 13 Monitor System. Problems may be run using either the binary object or source program deck. The binary object deck is preferred since no compilation time is needed and the probability of damage to the source deck is eliminated. The deck setup for the binary object program is described below. The deck setup with source decks is identical except the FORTRAN source language subroutine decks are substituted for binary object decks.

TAPAT PROGRAM DECK SETUP

1) An accounting card (dependent on computer installation)
2) A job card, $ JOB in columns 1-4
3) A pause card, $PAUSE in columns 1-6 (this card is required to permit the IBM 7094 operator to mount a master cross section tape and should be deleted if no master tape is used).
4) An execute card $EXECUTE in columns 1-8 and IBJOB in columns 16-20.
5) An IBSYS job card, $IBJOB in columns 1-6 and GO, ALTIO in columns 16-27.
6) The main subroutine binary object deck
7) An overlay origin card, $ORIGIN in columns 1-7 and ALPHA, SYSUT3 in columns 16-27.
8) The binary object deck for the control link program, for FLUX EDIT and ADDICT subprograms (Subroutine C0013)
9) An overlay origin card $ORIGIN in columns 1-7 and BETA, SYSUT3 columns 16-26.
10) The binary object deck for FLUX EDIT
11) Same as 9 above
12) The binary object decks for the first overlay of ADDICT (Subroutines C023, MIXX, INPR, SCHECK, SEARCH)

13) Same as 9 above

14) The binary object decks for the second overlay of ADDICT (Subroutines C033, FLUX, CONN, SOURCE)

15) Same as 9 above

16) The binary object deck for the third overlay of ADDICT (Subroutine C043)

17) An overlay origin card the same as 7 above

18) The binary object deck for the control link program of MISPHT, (Subroutine C0053)

19) An overlay origin card, $ORIGIN in columns 1-7 and GAMMA, SYSUT3, in columns 16-27

20) The binary object decks for the first overlay of MISPHT (Subroutines C053, MIXX5, INPR5, SEARC5, SCHCK5)

21) Same as 19 above

22) The binary object decks for the second overlay of MISPHT (Subroutines C063, OPINT, SETUP, ALQS, AQSJL, FACTOR, BUNDRY, MTXSET)

23) Same as 19 above

24) The binary object decks for the third overlay of MISPHT (Subroutine C073, FLUX7, CONV7, SOURCB)

25) Same as 19 above

26) The binary object deck for the fourth overlay of MISPHT (Subroutine C003)

27) An overlay origin card same as 7 above

28) The binary object deck for the control link program of MIST (Subroutine C0093)

29) An overlay origin card, $ORIGIN in columns 1-7 and SIGMA, SYSUT3, in columns 16-27

30) The binary object decks for the first overlay of MIST (Subroutines C03, MIXXC, SEARCC, INPRC, SCHECC)

31) Same as 29 above

32) The binary object decks for the second overlay of MIST (Subroutines C103, OPINTC, SETOPC, ALQSC, MTXSFC, AQSJLC, FACTOC, BUNDRC)

33) Same as 29 above

34) The binary object decks for the third overlay of MIST (Subroutines C113, FLUX, SOURCE, CONVC)

35) Same as 29 above

36) The binary object deck for the fourth overlay of MIST (Subroutine C123)

37) Same as 7 above

38) The binary object deck for the control link program of TOPIC, (Subroutine C0133)

39) An overlay origin card, $ORIGIN in columns 1-7 and PI, SYSUT3, in columns 16-27

40) The binary object decks for the first overlay of TOPIC (Subroutines C133, MIXXD, SCHECD, SEARCD, INPRD)

41) Same as 39 above

42) The binary object decks for the second overlay of TOPIC (Subroutines C143, MIXSEL, SSET, FACTOD, MIXSED, BUNDRD)

43) Same as 39 above

44) The binary object decks for the third overlay of TOPIC (Subroutine C153, FLUXD, SOURCD, CONVD, HIMODE)

45) Same as 39 above

46) The binary object deck for the fourth overlay of TOPIC (Subroutine C163)

47) An entry control card, $ENTRY in columns 1-6

48) A data control card, $DATA in columns 1-5

49) TAPAT Problem Data
    a) TAPAT control card
    b) Alphanumeric Card
    c) Fixed point data
    d) Floating print data

50) Appropriate end of file cards

The above program deck setup is placed on tape using an IBM Model 1401 or IBM Model 360/30 Computer to manufacture a standard system input tape. Once the input has been written on tape, the machine operation is standard and the only operator action required is the mounting and dismounting of a master cross section tape if desired.

SECTION

7.0 REFERENCES

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