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Final Report

DMM: A MULTIGROUP, MULTIREGION, ONE-SPACE-DIMENSIONAL COMPUTER PROGRAM USING NEUTRON DIFFUSION THEORY

Part I - The Theory

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CONTENTS

FOREWORD

This document is submitted in partial fulfillment of the final technical report requirements of Part I, para. E.3., item III, of the Statement of Work of U. S. Air Force Contract AF33(616)-6097. The report is presented in three parts: I - "The Theory," contained herein; II - "DMM Program Description;" the third part consists of the Uniservo tape(s) and two copies of the program on IBM cards.

A basic library of cross sections for DMM has been developed by D. L. Kavanagh and is presented in American-Standard Report ATL-A-106, "Cross Section Library for DMM: A Multigroup, Multiregion, One-Space-Dimensional Computer Program Using Neutron Diffusion Theory" (Secret-Restricted Data).

ACKNOWLEDGEMENT

The basic DMM computer code was originally planned in a cooperative effort by members of the staff of Advanced Technology Laboratories, a Division of American-Standard; Electrodata Division of Burroughs Corporation; the Missiles and Space Division of Lockheed Aircraft Corporation; International Business Machines Corporation; the Atomic Power Equipment Division of General Electric Company; and Remington Rand Corporation. Among those who contributed were Joel Franklin, Jack Rosengren, Martin Walt, Thomas Wilder III, Lou G. Kelly, Robert J. Levit, and Edward J. Leshan. The initial description of the program was presented in American-Standard Report ASAE-4 ("A Multigroup, Multi-region, One-Space-Dimensional Program Using Neutron Diffusion Theory," April 1957) by Edward J. Leshan and Joel Franklin. Versions of the diffusion portion of the program have been coded for the IBM 650 by Robert J. Levit of IBM, for the IBM 704 by Larry Blue of Atomics International, for the Remington Rand 1103 by David M. Williams of Lockheed, and for the Datatron 205 by Joel Franklin.

The version described in this report was designed and programmed for the Remington Rand 1103A by the authors at Advanced Technology Laboratories under contract with Wright Air Development Division. Technical surveillance was by Captain John E. Brooke. Lockheed Aircraft Corporation contributed computer time for program checking.

ABSTRACT

DMM is a program using one-space-dimensional multigroup diffusion theory to calculate the reactivity or critical conditions and flux distribution of a multiregion reactor. Calculations of fission-produced xenon and samarium and time variation due to production and depletion of isotopes are an essential part of this program. The adjoint fluxes may also be computed, and the program includes the calculation of the nuclear constants from fairly simple input combined with a library of cross sections. The present code is written for the Remington Rand 1103A. Operating instructions are presented in Part II of this report.

I. INTRODUCTION

DMM is a computer program whose primary purpose is the calculation of the spatial and energy distribution of the flux of neutrons in a spherical, cylindrical, or slab reactor and of the reactivity of this system. As auxiliary programs intimately associated with this purpose, DMM includes:

1) The calculation of multigroup cross sections, using interpolated estimates of the flux within an energy group to weight what is essentially a point cross section table.
2) A burnup routine, using the fluxes calculated by the main program to compute the consumption and production of reactor materials in finite time steps. After calculating the amount of an absorbing material that must be added to maintain the multiplication at unity, the program computes new group constants and returns to the main program to compute new fluxes and a new reactivity.
3) The calculation of the xenon and samarium distribution from the fluxes, recomputation of the group constants using these added materials, followed by return to the main program to calculate new fluxes and multiplication with the new group constants. The xenon and samarium distributions are computed for equilibrium or for a given time after shutdown.
4) Calculation of the adjoint fluxes, using the main flux program with altered nuclear constants.
5) Iteration on any one of several reactor parameters, such as concentration of any one of the elements in any one of the regions, size of one of the regions, and transverse leakage. This procedure obtains the value of the chosen parameter at which the reactivity is equal to a given value.

The program is written in such a way that the various separate routines may be linked together in any one of several ways to satisfy the requirements of a particular problem.

II. THE DIFFUSION EQUATION

A. General Discussion

The principal calculation is the solution of a diffusion theory approximation for the multiplication and neutron flux in a nuclear system:

$$\nabla[D(r,E)\,\nabla\phi(r,E)] - \Sigma_t(r,E)\,\phi(r,E)$$

$$+\sum_A \chi_{in_A}(r,E) \int_E^{E_{max}} \Sigma_{in_A}(r,E')\,\nu_{in_A}(r,E')\,\phi(r,E')\,\frac{dE'}{X_{in_A}(r,E')}$$

$$+\sum_A \int_E^{\min(E/\alpha_A,\,E_{max})} \frac{\Sigma_{s_A}(r,E')\,\phi(r,E')\,dE'}{(1-\alpha_A)\,E'}$$

$$= -\frac{\chi_f(r,E)}{k} \sum_A \int_{E_{min}}^{E_{max}} \Sigma_{f_A}(r,E')\,\nu_{f_A}(r,E')\,\phi(r,E')\,dE' \quad . \qquad (1)$$

In addition to the diffusion approximation, several other assumptions have been made in writing equation 1.

The second term covers inelastic scattering and implies that $\chi_{in_A}(r,E)\,dE$, the probability that a neutron absorbed at a higher energy E' will be emitted with an energy between E and E + dE (if an inelastic collision takes place), is dependent on E' only in that it is zero for E > E'. The divisor $X_{in_A}(R,E')$ is given by

$$X_{in_A}(r,E') = \int_{E_{min}}^{E'} \chi_{in_A}(r,E'')\,dE'' \qquad (2)$$

and is included to normalize the truncated $\chi_{in_A}(r,E)$.

The third term covers elastic scattering and is exact except for the assumption that scattering is isotropic in the center of mass system. In the rare cases where this is

significant, nonisotropic components can be included by replacing the scatterer with several scatterers of different atomic weight.

The terms in equation 1 not described above may be defined as follows:

r = the single spatial coordinate over which the integration of equation 1 is performed in detail. In the case of a sphere, r is the distance from the center; in cylindrical calculations it is the perpendicular distance from the axis. Finally, in the case of slab geometry, it is the single Cartesian coordinate being investigated.

E = the energy of the neutrons.

$D(r,E)$ = the neutron diffusion coefficient.

$\phi(r,E)$ = the neutron flux density.

$\Sigma_t(r,E)$ = the macroscopic total cross section plus a leakage cross section accounting for leakage in directions other than r.

$\Sigma_{in_A}(r,E)$ = the macroscopic inelastic scattering cross section. An inelastic event is defined as a collision of the types (n, n'), (n, 2n), (n, 3n), etc.

$\nu_{in_A}(r,E)$ = the number of neutrons emitted per inelastic collision with the A^{th} isotope.

α_A = the maximum fractional energy loss for a neutron colliding with the A^{th} isotope.

Σ_{s_A} = the macroscopic elastic scattering cross section for the A^{th} isotope.

$\chi_f(r,E)dE$ = the probability that a neutron emitted after a fission has energy in the range E to E + dE.

$\mathcal{K}$ = the effective multiplication.

Σ_{f_A}, ν_{f_A} = the macroscopic fission cross section and the number of neutrons emitted per fission, respectively, for the A^{th} isotope.

B. The Multigroup Method

If we define energy ranges E^i to E^{i+1} for i = 1, 2, ... I and integrate equation 1 over these ranges, we obtain a set of equations, one for each energy group.

$$-\nabla[D^i(r)\nabla\phi^i(r)] + T^i(r)\,\phi^i(r) = H^i(r) \tag{3}$$

where $$H^i(r) = \sum_{j=1}^{i-1} T^{ij}(r)\,\phi^j(r) + \chi_f^i\,P(r), \tag{4}$$

and $$P(r) = \frac{1}{\mathcal{K}} \sum_{j=1}^{I} F^j(r)\,\phi^j(r) \tag{5}$$

The nuclear constants D^i, T^i, T^{ij}, χ_f^i, F^i, Σ_f^i, and the flux ϕ^i are related to the functions in equation 1 by integration formulas as described in section III. Briefly, they are flux-weighted averages of the energy-dependent cross sections averaged over the range E_i to E_{i+1}.

C. The Spatial Integration

We further define N + 1 mesh points r_0, r_1, $r_2 \ldots r_N$ at which the functions of equations 3, 4, and 5 are defined. These mesh points may be grouped into regions in each of which the nuclear properties are independent of position. That is, $T^i(r) = {}^kT^i$ for $R_{k-1} \leq r \leq R_k$, etc., where R_k and R_{k-1} each coincide with some r_n and are the outer and inner points, respectively, of some geometric region. In this program, the mesh spacing is constant within each region but may vary from region to region. That is, $r_{n+1} - r_n = r_{n'+1} - r_{n'}$, if for some k,

$$R_{k-1} \leq r_n < r_{n+1} \leq r_{n'} < r_{n'+1} \leq R_k \quad .$$

There are R regions, where k = 1, 2, 3....R.

Setting ρ = 0, 1, or 2 for planar, cylindrical, and spherical geometries, respectively, we obtain:*

$$-a_n^i \phi_{n-1}^i + b_n^i \phi_n^i - c_n^i \phi_{n+1}^i = d_n^i \quad . \quad (n = 0, 1, 2 \ldots N) \tag{6}$$

$$\left.\begin{aligned} a_n^i &= {}^{k-}D^i \frac{r_{n-1/2}^{\rho}}{\Delta r_{n-}} \quad . \\ b_n^i &= a_n^i + c_n^i + 1/2\ r_n^{\rho}\ \Delta r_{n-}\ {}^{k-}T^i + 1/2\ r_n^{\rho}\ \Delta r_{n+}\ {}^{k+}T^i \quad . \\ c_n^i &= {}^{k+}D^i \frac{r_{n+1/2}^{\rho}}{\Delta r_{n+}} \quad . \\ d_n^i &= 1/2\ r_n^{\rho}\ \Delta r_{n-}\ H_{n-}^i + 1/2\ r_n^{\rho}\ \Delta r_{n+}\ H_{n+}^i \quad . \end{aligned}\right\} (n = 1, 2 \ldots N-1) \tag{7}$$

* For a derivation of these equations, see "RBU: A Combined Monte Carlo Reactor Burnup Program for the IBM 709," Advanced Technology Laboratories, a Division of American-Standard, ATL-A-101, 30 September 1959, pp 85-88.

Here,

$$
\left.
\begin{aligned}
r_{n-1/2} &= 1/2(r_{n-1} + r_n) \quad ; \\
\Delta r_{n-} &= r_n - r_{n-1} \quad ; \\
\Delta r_{n+} &= r_{n+1} - r_n \quad ; \\
H^i_{n-} &= \sum_{j=1}^{i-1} {}^{k-}T^{ij}\ \phi^j_n + \chi^i_f P_{n-} \quad ; \\
H^i_{n+} &= \sum_{j=1}^{i-1} {}^{k+}T^{ij}\ \phi^j_n + \chi^i P_{n+} \quad ;
\end{aligned}
\right\} \quad (8a)
$$

$$
\left.
\begin{aligned}
P_{n-} &= \frac{1}{\mathcal{A}} \sum_{j=1}^{I} {}^{k-}F^j\ \phi^j_n \quad ; \\
P_{n+} &= \frac{1}{\mathcal{A}} \sum_{j=1}^{I} {}^{k+}F^j\ \phi^j_n \quad ;
\end{aligned}
\right\} \quad (8b)
$$

k- refers to the material at the left of mesh point n;

k+ refers to the material at the right of mesh point n.

For mesh points that do not correspond to the boundaries between regions, (7) is somewhat simpler, since for these points

$$\Delta r_{n-} = \Delta r_{n+},\ {}^{k-}T^i = {}^{k+}T^i,\ {}^{k+}D^i = {}^{k-}D^i,\ {}^{k-}T^{ij} = {}^{k+}T^{ij},\ {}^{k-}F^j = {}^{k+}F^j \quad .$$

D. Boundary Conditions

At the boundaries of the mesh, r_0 and r_N, the equations for a^i_n, b^i_n, c^i_n, and d^i_n are modified to agree with the boundary conditions. These are

$$
\begin{aligned}
-[1 - B^i_0]\ {}^1D^i\ \frac{\phi^i_1 - \phi^i_0}{\Delta r_{0+}} + B^i_0\ \phi^i_0 + D\nabla^2\phi\ \frac{\Delta r_0^{\,2}}{2} &= 0 \quad ; \\
[1 - B^i_N]\ {}^RD^i\ \frac{\phi^i_N - \phi^i_{N-1}}{\Delta r_{N-}} + B^i_N\ \phi^i_N + D\nabla^2\phi\ \frac{\Delta r_N^{\,2}}{2} &= 0 \quad ;
\end{aligned}
\quad (9)
$$

which correspond to the physical boundary conditions:

$$
\begin{aligned}
-[1 - B_0(E)]\ D(0,E)\ \nabla\phi(0,E) + B_0(E)\ \phi(0,E) + D(0,E)\nabla^2\phi(0,E) &= 0 \quad ; \\
[1 - B_N(E)]\ D(R,E)\nabla\phi(N,E) + B_N(E)\ \phi(N,E) + D(R,E)\nabla^2\phi(R,E) &= 0 \quad .
\end{aligned}
\quad (10)
$$

These equations permit solutions corresponding to flux zero at an extrapolated end point, symmetrical or nonsymmetrical slabs, an infinite nonmoderating reflector, or to other values of the logarithmic derivative at the boundary. The most commonly used boundary conditions will presumably be $B_0^i = 0$, $B_N^i = 0.319$.*

Equations 9 lead to the following equations for n = 0 and N.

$$\left.\begin{aligned} a_0^i &= 0 \\ b_0^i &= c_0^i + B_0^i \Delta r_{0+} + \tfrac{1}{2}(1 - B_0^i)\, {}^1T^i (\Delta r_{0+})^2 \\ c_0^i &= (1 - B_0^i)\, {}^1D^i \\ d_0^i &= \tfrac{1}{2} H_0^i (1 - B_0^i)(\Delta r)^2 \end{aligned}\right\} \quad (11)$$

$$\left.\begin{aligned} a_N^i &= (1 - B_N^i)\, {}^RD^i \\ b_N^i &= a_N^i + B_N^i \Delta r_{N-} + \tfrac{1}{2}(1 - B_N^i)\, {}^RT^i (\Delta r_{N-})^2 \\ c_N^i &= 0 \\ d_N^i &= \tfrac{1}{2}(1 - B_N^i) H_N^i (\Delta r_{N-})^2 \end{aligned}\right\} \quad (12)$$

E. Numerical Procedures

Since the boundary conditions (equations 11 and 12) apply at opposite ends of the mesh, the solution of equations 6 and 7 subject to them requires some special device. We define p_n^i and q_n^i by

$$\phi_n^i = p_n^i \phi_{n+1}^i + q_n^i \quad . \quad (13)$$

---

* The use of $B_N^i = 0.319$ instead of the more customary zero permits the use of actual reactor dimensions and automatically sets the extrapolation to 0.71λ with its appropriate energy dependence through the energy dependence of λ.

Substituting equation 13 into equation 6 gives as a solution

$$p_n^i = \frac{c_n^i}{b_n^i - a_n^i p_{n-1}^i} ; \quad q_n^i = \frac{d_n^i + a_n^i q_{n-1}^i}{b_n^i - a_n^i p_{n-1}^i} . \tag{14}$$

If the source H_n^i is known, it is possible to calculate the p_n^i and q_n^i beginning with n = 0. By substituting these values in equation 13, the ϕ_n^i may then be evaluated. Since

$$T_n^{ij} = 0, \ (i \leq j) \tag{15}$$
(Scattering transfer only from some group j to a lower energy group i.)

H_n^i can be calculated from P_n without any knowledge of the ϕ_n^i. Thus, if the P_n are known, the ϕ_n^i can be calculated, beginning with i = 1 and proceeding, one group at a time, to i = I.

Having computed the ϕ_n^i, the P_n are computed by equations 8b.

$$\mathscr{E} = \frac{1}{VP_0Q} \sum_n \sum_i \left({}^{k-}\Sigma_f^i \Delta V_{n-} + {}^{k+}\Sigma_f^i \Delta V_{n+} \right) \phi_n^i , \tag{16}$$

where

$$\left.\begin{aligned} \Delta V_{n-} &= \begin{cases} 1/2 \, \Delta r_{n-} & \text{for } \rho = 0 , \\ \pi r_n \Delta r_{n-} & \text{for } \rho = 1 , \\ 2\pi r_n^2 \Delta r_{n-} & \text{for } \rho = 2 ; \end{cases} \\ \Delta V_{n+} &= \begin{cases} 1/2 \, \Delta r_{n+} & \text{for } \rho = 0 , \\ \pi r_n \Delta r_{n+} & \text{for } \rho = 1 , \\ 2\pi r_n^2 \Delta r_{n+} & \text{for } \rho = 2 ; \end{cases} \end{aligned}\right\} \tag{17}$$

$$\left.\begin{aligned} \Delta V_n &= \Delta V_{n-} + \Delta V_{n+} ; \\ \Delta V_{0-} &= 0 ; \\ \Delta V_{N+} &= 0 ; \\ V &= \sum_{n=0}^{N} \Delta V_n ; \\ \Delta r_{0-} &= \Delta r_{N+} = 0 . \end{aligned}\right\} \tag{18}$$

The effect of this treatment is that at each iteration the fluxes and sources are normalized to an average value of $P_0 Q$ fissions per unit volume, where Q = the operating power density in kw/cm^3 of reactor,* P_0 = number of fissions/kw-sec = 3.12×10^{13}. The flux density, then, is in neutron centimeters per cubic centimeter per second per unit energy at an average position in the transverse space variable.

Using the values of the P_n computed by equation 8b, the program calculates a new set of ϕ_n^i and continues the iterative process until agreement between successive iterates of P_n and k indicates satisfactory convergence. The criterion for satisfactory convergence is that $\left| \frac{{}^tP_n - {}^{t-1}P_n}{{}^tP_n} \right| < \epsilon_2$ for all n and that $\left| {}^tk - {}^{t-1}k \right| < \epsilon_1$.

In addition to these tests, the maximum number of iterations of the diffusion calculation for a particular problem may be controlled by the user through the control information input.

In order to accelerate the rate of convergence, $\tilde{P}_n$ was used in equation 8a instead of P_n:

$$ {}^t\tilde{P}_n = [{}^tP_n + \omega({}^tP_n - {}^{t-1}\tilde{P}_n)] \quad , \tag{19}$$

where the presubscript, t, is the iteration number and ω is an input constant. Should equation 19 yield a negative value for any n, that particular ${}^t\tilde{P}_n$ is set equal to zero. Methods of determining the best value of ω are discussed elsewhere.** On the first iteration, it is necessary to generate a set. This set, obtained on the assumption of a flat power distribution, is $P_n = 2.5\ P_0 Q$.

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* Note that this power density differs from the power per unit volume of core by the factor (core volume/reactor volume).

** See, for example: E. L. Wachspress, "Iterative Methods of Solving Elliptic-Type Differential Equations," KAPL 1333 (1955).

III. THE NUCLEAR CONSTANTS

A. General Discussion

The integration of equation 1 leads to the following definitions for the functions appearing in equations 3, 4, and 5.

$$D^i \equiv \left[\int_{E_{i+1}}^{E_i} D(E)\,\phi(E)\,dE \right] \Big/ \phi^i\,(E_i - E_{i+1}) \quad . \tag{20}$$

$$T^{i\,\dagger} = \int_{E_{i+1}}^{E_i} \left\{ \Sigma_t(E)\phi(E) - \sum_A \chi_{in_A}(E) \int_E^{E_i} \Sigma_{in_A}(E')\,(E)\,\frac{dE'}{X_{in_A}(E')} \right.$$

$$\left. - \sum_A \int_E^{\min(E/\alpha_A, E_i)} \frac{\Sigma_{s_A}(E')}{(1-\alpha_A)E'}\,\phi(E')\,dE' \right\} dE \Big] \Big/ \phi^i(E_i - E_{i+1})$$

$$- [B^2 D]^i \tag{21}$$

$$T^{ij\,\ddagger} \equiv \int_{E_{i+1}}^{E_i} \left\{ \sum_A \chi_{in_A}(E) \int_{E_{j+1}}^{E_j} \Sigma_{in_A}(E')\,\nu_{in_A}(E')\phi(E')\,\frac{dE'}{X_{in_A}(E')} \right.$$

$$\left. + \sum_A \int_{E_{j+1}}^{\min(E/\alpha_A, E_j)} \frac{\Sigma_{s_A}(E')}{(1-\alpha_A)E'}\,\phi(E')dE' \right\} dE \Big] \Big/ \phi^j(E_i - E_{i+1}) \text{ if } j < i \text{ and}$$

$$T^{ij} = 0 \text{ if } j \geq i. \tag{22}$$

---

† See equation 37 for the way the second and third terms of T^i are actually computed.

‡ See equation 33a for the way the variable upper limit is actually included in the second term of T^{ij}.

$$\chi_f^i \equiv \left[\int_{E_{i+1}}^{E_i} \chi_f(E)dE\right] \Big/ (E_i - E_{i+1}) \quad . \tag{23}$$

$$F^j \equiv \left[\int_{E_{j+1}}^{E_j} \Sigma_f(E)\nu_f\, \phi(E)dE\right] \Big/ \phi^j \quad . \tag{24}$$

$$\Sigma_f^i = \left[\int_{E_{i+1}}^{E_i} \Sigma_f(E)\, \phi(E)dE\right] \Big/ \phi^i \quad . \tag{24a}$$

$$\phi^i \equiv \int_{E_{i+1}}^{E_i} \phi(E)dE \Big/ (E_i - E_{i+1}) \quad . \tag{25}$$

$(B^2D)^i$ is the perpendicular leakage cross section which normally is an input constant. Although equations 20 through 25 are easily derived by integration of equation 1, if one assumes an energy-independent buckling, a different equation can be derived for D^i by integrating the transport equation to obtain a multigroup transport equation and deriving a diffusion approximation to this. The results obtained from the two definitions are often not very different from each other; in this program, the second more convenient and conventional definition is used.

$$D^i \equiv \frac{1}{3\Sigma_{tr}^i} \equiv \frac{1}{3}\left\{\left[\int_{E_{i+1}}^{E_i} \Sigma_{tr}(E)\, \phi(E)dE\right] \Big/ \phi^i(E_i - E_{i+1})\right\}^{-1} \tag{20a}$$

B. Flux Weighting

The calculation of these quantities must use different equations, since $\phi(E)$ is not known and since the above equations imply a computation at each mesh point--an excessive amount of work. As a compromise, the function ${}^k\psi(E)$ is used in place of $\phi(E)$ in equations 20 through 24. Equation 25 need not be performed at all. ${}^k\psi(E)$ is obtained from a set of ϕ^i by integrating the ϕ_n^i over regions of uniform composition and interpolating. Thus, if

$${}^k\phi^i \equiv \sum_{N_{k-1}}^{N_k} \phi_n^i\, \Delta V_n \quad , \tag{26}$$

where k indicates the k^{th} region,

$$ {}^{k}\psi^{i}(E) = {}^{k}C_1^{i} + \frac{{}^{k}C_2^{i}}{E} + {}^{k}C_3^{i} \times E \quad . \qquad E_{i+1} \leq E < E_i \quad . \tag{27} $$

The coefficients are defined by

$$ {}^{k}\phi^{i-1} = {}^{k}C_1^{i} + \frac{{}^{k}C_2^{i}}{E_{i-1/2}} + {}^{k}C_3^{i} \quad E_{i-1/2} \quad ; $$

$$ {}^{k}\phi^{i} = {}^{k}C_1^{i} + \frac{{}^{k}C_2^{i}}{E_{i+1/2}} + {}^{k}C_3^{i} \quad E_{i+1/2} \quad ; \tag{28} $$

$$ {}^{k}\phi^{i+1} = {}^{k}C_1^{i} + \frac{{}^{k}C_2^{i}}{E_{i+3/2}} + {}^{k}C_3^{i} \quad E_{i+3/2} \quad . $$

$$ E_{i+1/2} \equiv \frac{E_{i+1} + E_i}{2} \quad . $$

The assumption of a particular functional form (equation 27) for $\psi(E)$ makes possible the performance of all the integrations involved in equations 20a through 24 for each isotope for a given group structure, that is, for a given set of E_i at the time the group structure is first defined. In order to do this, the microscopic equivalents of the macroscopic cross sections used in (20) through (25)* are defined as follows:

$$ {}^{k}T^{i} = \sum_A {}^{k}N_A \; {}^{k}t_A^{i} + {}^{k}(B^2D)^{i} \quad ; $$

$$ {}^{k}\Sigma_{tr}^{i} = \sum_A {}^{k}N_A \; {}^{k}\sigma_{tr_A}^{i} \quad ; $$

$$ {}^{k}T^{ij} = \sum_A {}^{k}N_A \; {}^{k}t_A^{ij} \; \frac{(E_j - E_{j+1})}{(E_i - E_{i+1})} \quad ; \tag{29} $$

$$ {}^{k}F^{i} = \sum_A {}^{k}N_A \; {}^{k}f_A^{i} \; (E_i - E_{i+1}) \quad ; $$

$$ {}^{k}\Sigma_{f}^{i} = \sum_A {}^{k}N_A \; {}^{k}\sigma_{f_A}^{i} \; (E_i - E_{i+1}) \quad . $$

---

* See section IV for the modification of equation 29 that is actually used.

Here, the index A refers to a particular isotope, and ${}^{k}N_{A}$ is the concentration of that isotope in region k.

The region superscript on the microscopic cross sections indicates that they have been weighted by the ${}^{k}\psi^{i}$ in the process of obtaining group values from the more detailed dependence of the nuclear properties on energy.

This program uses a set of cross sections, called the basic library, which describes the detailed dependence of the cross section of each isotope on energy. Among the nuclear data specified in the basic library are $\sigma_s(E)$, $\sigma_c(E)$, $\sigma_f(E)$, $\sigma_{in}(E)$, $\nu_f(E)$, $\nu_{in}(E)$, $X(E)$, $\bar{\mu}_o(E)$, and α. With these and the definition

$$\sigma_{tr} = \sigma_s(1-\bar{\mu}_o) + \sigma_c + \sigma_f + \sigma_{in} \quad , \tag{30}$$

the microscopic analogues to the integrations of (20a) through (24) may be carried out provided the weighting functions ${}^{k}\psi^{i}(E)$ are available. Since, however, these weighting functions are always to be of the form of equation 27, it is convenient to define three separate microscopic cross sections for each of those used in (29). That is if

$$\begin{aligned}
{}^{k}t_{A}^{i} &= \frac{1}{{}^{k}C^{i}}\left[{}^{k}C_1^{i}\ {}^{i}t_{1_A} + {}^{k}C_2^{i}\ {}^{i}t_{2_A} + {}^{k}C_3^{i}\ {}^{i}t_{3_A}\right] \quad ; \\
{}^{k}\sigma_{tr_A}^{i} &= \frac{1}{{}^{k}C^{i}}\left[{}^{k}C_1^{i}\ {}^{i}\sigma_{tr_{1_A}} + {}^{k}C_2^{i}\ {}^{i}\sigma_{tr_{2_A}} + {}^{k}C_3^{i}\ {}^{i}\sigma_{tr_{3_A}}\right] \quad ; \\
{}^{kij}t_{A} &= \frac{1}{{}^{k}C^{j}}\left[{}^{k}C_1^{j}\ {}^{ij}t_{1_A} + {}^{k}C_2^{j}\ {}^{ij}t_{2_A} + {}^{k}C_3^{j}\ {}^{ij}t_{3_A}\right] \quad ; \text{ etc.},
\end{aligned} \tag{31}$$

where $${}^{k}C^{i} = {}^{k}C_1^{i}(E_i - E_{i+1}) + {}^{k}C_2^{i}\ln\frac{E_i}{E_{i+1}} + \frac{1}{2}{}^{k}C_3^{i}(E_i^{\,2} - E_{i+1}^{\,2}) \quad ,$$

then ${}^{i}t_{1_A}$, ${}^{i}t_{2_A}$ and ${}^{i}t_{3_A}$ may be obtained from the basic library and the energy group structure independent of the ${}^{k}C_1^{i}$, ${}^{k}C_2^{i}$, ${}^{k}C_3^{i}$.

C. Microscopic Group Constants

When the program is given an energy group structure and a list of isotopes that will be required, it computes the following group constants.

$$\begin{Bmatrix} \sigma^{i}_{tr_{1_A}} \\ \sigma^{i}_{tr_{2_A}} \\ \sigma^{i}_{tr_{3_A}} \end{Bmatrix} = \int_{E_{i+1}}^{E_i} \sigma_{tr_A}(E) \begin{Bmatrix} 1 \\ \frac{1}{E} \\ E \end{Bmatrix} dE. \qquad (32)$$

$$\begin{Bmatrix} t^{ij}_{1_A} \\ t^{ij}_{2_A} \\ t^{ij}_{3_A} \end{Bmatrix} = \int_{E_{i+1}}^{E_i} \left[\chi_{in_A}(E) \int_{E_{j+1}}^{E_j} \sigma_{in_A}(E') \, \nu_{in_A}(E') \begin{Bmatrix} 1 \\ \frac{1}{E'} \\ E' \end{Bmatrix} \frac{dE'}{X_A(E')} \right.$$

$$\left. + \int_{E_{j+1}}^{\min(E/\alpha_A, E_j)} \frac{\sigma_{s_A}(E')}{(1-\alpha_A)E'} \begin{Bmatrix} 1 \\ \frac{1}{E'} \\ E' \end{Bmatrix} dE' \right] dE. \qquad (33)$$

The cross section t'^{ij} is also computed by an equation identical to (33) except for the suppression of ν_{in}.

To simplify the computation, the variable upper limit in (33) is eliminated and the elastic scatter term replaced by

$$\epsilon(E, E_j, \alpha) \int_{E_{j+1}}^{E_j} \frac{\sigma_{s_A}(E')}{(1-\alpha_A)E'} \begin{Bmatrix} 1 \\ \frac{1}{E'} \\ E' \end{Bmatrix} dE' \quad ,$$

where
$$\epsilon(E, E_j, \alpha) = \frac{\frac{E}{\alpha} - E_{j+1}}{E_j - E_{j+1}} \quad \text{if } E_{j+1} < \frac{E}{\alpha} < E_j \quad ;$$

$$= 1 \text{ if } \frac{E}{\alpha} > E_j \quad ; \qquad (33a)$$

$$= 0 \text{ if } \frac{E}{\alpha} < E_{j+1} \, .$$

$$\begin{Bmatrix} f^j_{1_A} \\ f^j_{2_A} \\ f^j_{3_A} \end{Bmatrix} = \nu^j_{f_A} \int_{E_{j+1}}^{E_j} \left[\sigma_{f_A}(E) \begin{Bmatrix} 1 \\ \frac{1}{E} \\ E \end{Bmatrix} dE \right] . \tag{34}$$

$$\begin{Bmatrix} \sigma^i_{f_{1_A}} \\ \sigma^i_{f_{2_A}} \\ \sigma^i_{f_{3_A}} \end{Bmatrix} = \int_{E_{i+1}}^{E_i} \left[\sigma_{f_A}(E) \begin{Bmatrix} 1 \\ \frac{1}{E} \\ E \end{Bmatrix} dE \right] . \tag{35}$$

$$\begin{Bmatrix} \sigma^i_{c_{1_A}} \\ \sigma^i_{c_{2_A}} \\ \sigma^i_{c_{3_A}} \end{Bmatrix} = \int_{E_{i+1}}^{E_i} \left[\sigma_{c_A}(E) \begin{Bmatrix} 1 \\ \frac{1}{E} \\ E \end{Bmatrix} dE \right] . \tag{36}$$

$$t^i_{\ell A} = \sigma^i_{f_{\ell A}} + \sigma^i_{c_{\ell A}} + \sum_{j=i+1}^{I} t'^{ji}_{\ell A} . \tag{37}$$

To repeat, the isotopic group constants of (32) through (37) and, in addition χ^i_f, are computed when an energy group structure is defined and a list of isotopes required for the problem specified. The program may examine an old microscopic group tape and compute the group constants only for those isotopes needed which are not already on the old tape.

If a set of $^k\phi^i$ are available, the program may then compute the $^kC^i_\ell$ by solving equation 28 and from them the microscopic constants of (29) by means of (31). Two additional cross sections $^k\sigma^i_{f_A}$ and $^k\sigma^i_{c_A}$ are needed for burnup calculation and are computed in the same way.

The program tests the computation of each parameter evaluated in equation 31; if any are negative, they are recomputed with ${}^{k}C_{2}^{i} = {}^{k}C_{3}^{i} = 0$.

The definitions in (28) are modified in a simple way in the case of the first and last groups:

$$\begin{aligned} \phi^{0} &\equiv 1 \quad ; \\ E_{1/2} &\equiv E_{1} \quad ; \\ \phi^{I+1} &\equiv 1 \quad ; \\ E_{I+3/2} &\equiv E_{i+1} \quad . \end{aligned} \tag{38}$$

The choice of ϕ's = 1 causes the weighting functions C_2 and C_3 evaluated in the initial case to be identically equal to zero.

The calculation of the neutron spectrum within the thermal group is presumably performed by some other program--either a Maxwellian is assumed or some method such as Wigner-Wilkins is used. At any rate, the averaging over this thermal group must at present be done externally to DMM. The effect of these cross sections on the thermal group cross sections is then established by DMM through an appropriate choice of the low-energy entries in the basic library.*

D. The Basic Library

The detailed dependence of the nuclear constants in the basic library on energy implied in the integrations of equations 32 through 37 is obtained by specifying the values at a large number of energies. These energy values are chosen to be appropriate to the most economical, yet accurate representation for each individual isotope without regard to the values used for other isotopes.

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* Modification of DMM to include the determination of a thermal spectrum and evaluation of thermal group cross sections that have been averaged over it is certainly practical. An alternative approach that may be superior is to provide in the nuclear constants routine for a special scattering model near thermal energies, to add upscattering terms to the t^{ij} and T^{ij}, and then to treat several groups near thermal in the conventional way. In any case, it is usually necessary to have additional separate computations to deal with such effects as shelf shielding, resonances and near thermal scattering.

The ϕ_n^i used in the nuclear constant evaluation are the result of a previous iteration or stage of the calculation. Transfer to this cross section averaging routine may be made at some stage of the calculation when some of the auxiliary programs have caused a change in concentration of some components.

IV. SELF SHIELDING

Usually this code will be applied to a semi-homogeneous approximation of the actual reactor. For this reason, it may not be satisfactory to mix the isotopes according to their relative concentrations, as described in section III. This difficulty can be solved by multiplying the concentrations by self-shielding factors which are functions of energy and are the relative flux densities in the regions of a lattice cell.

In DMM, provision is made for several sets of self-shielding factors f_s^i, where p is the index of the set. With each isotope A in each region k, the set of self-shielding factors to be used is indicated by specifying the particular set through a value of ${}^k s_A$. If ${}^k s_A$ is zero, the program uses unity for the self-shielding factor for isotope A in region k. The f_s^i are inserted in equation 29, effectively producing a pseudo concentration that is energy dependent. For example:

$$ {}^k T^i = \sum_A {}^k N_A \, f^i_{{}^k s_A} \, {}^k t^i_A + {}^k (B^2 D)^i \quad . \tag{39} $$

V. XENON AND SAMARIUM ADDITION

Equilibrium, or shutdown xenon and samarium concentrations can be automatically computed and added to the contents of a region of the problem if the input indicates that this should be done. The calculation is made at a stage in the problem at which estimates of the P_n and ϕ_n^i are available.

The input required is

Δt_s - the time since shutdown in seconds ($\Delta t_s = 0$ gives equilibrium xenon and samarium concentration);

Q - the power density of the reactor in kw/cm^3 of reactor. *

The calculation makes use of the following constants:

P_0 - fissions/kw-sec = 3.12×10^{13}.

Y_{Xe} - Xe 135 atoms produced per fission = 3.0×10^{-3}.

Y_I - I 135 atoms produced per fission = 5.6×10^{-2}.

Y_{Pr} - Pr 149 atoms produced per fission = 1.4×10^{-2}.

λ_{Xe} - probability per second of decay of an Xe 135 atom = 2.1×10^{-5}.

λ_I - probability per second of decay of an I 135 atom = 2.9×10^{-5}.

λ_{Pr} - probability per second of decay of a Pr 149 atom = 4.1×10^{-6}.

$$k_{P'} = \sum_i {}^{k}\Sigma_f^i \; {}^{k}\phi^i \quad . \tag{40}$$

$$k\phi^i = \phi^i_{N_{k-1}} \Delta V_{N_{k-1}^+} + \sum_{n=N_{k-1}+1}^{N_k-1} \phi^i_n \Delta V_n + \phi^i_{N_i} \Delta V_{N_k^-} \quad ,$$

and $$kV = \Delta V_{N_{k-1}^+} + \sum_{n=N_{k-1}+1}^{N_k-1} \Delta V_n + \Delta V_{N_k^-} \quad ,$$

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* See footnote, page 10.

where ΔV_{n-}, ΔV_{n+} and ΔV_n are given by equation 17 and the average fission density in region k is then

$$k_p = \frac{k_{P'}}{k_V} \quad , \tag{41}$$

and the equilibrium concentration of Xe in region k is

$$k_{N_{Xe}^0} = \frac{(Y_I + Y_{Xe})\ k_p \times 10^{-24}}{\lambda_{Xe} + \sum_i {}^{k\,i}\sigma_{c_{Xe}}\ f^i_{k_{s_{Xe}}}\ \frac{k\,i}{k_V}\ (E_i - E_{i+1}) \times 10^{-24}} \quad . \tag{42}$$

where $f^i_{k_{s_{Xe}}}$ is the self-shielding factor associated with Xe in region k, group i.

At Δt_s seconds after shutdown, the concentration of Xe in region k is

$$k_{N_{Xe}}(\Delta t_s) = k_{N_{Xe}^0}\ e^{-\lambda_{Xe}\Delta t_s} + \frac{Y_I\ k_p \times 10^{-24}}{\lambda_1 - \lambda_{Xe}} \left[e^{-\lambda_{Xe}\Delta t_s} - e^{-\lambda_I \Delta t_s} \right]. \tag{43}$$

Similarly, the equilibrium concentration of Sm is

$$k_{N_{Sm}^0} = \frac{Y_{Pr}\ k_p}{\sum_i {}^{k\,i}\sigma_{c_{sm}}\ f^i_{k_{s_{Sm}}}\ \frac{k\,i}{k_V}\ (E_i - E_{i+1})} \quad , \tag{44}$$

and the concentration of Sm in region k at Δt_s seconds after shutdown is

$$k_{N_{Sm}}(\Delta t_s) = k_{N_{Sm}^0} + \frac{Y_{Pr}\ k_p \times 10^{-24}}{\lambda_{Pr}} \left(1 - e^{-\lambda_{Pr}\Delta t_s} \right) \quad . \tag{45}$$

Equations 43 and 45 apply of course only when the reactor has been in operation before shutdown for a sufficiently long period to establish equilibrium. Xenon and samarium concentrations during the approach to equilibrium may be computed by the burnup routine discussed in section VI.

VI. BURNUP

A. General

DMM may be used to compute, in conjunction with the calculations described above, the consumption and production of isotopes in each region during reactor operation. The procedure takes into account the spatial and energy variation of the neutron flux; also, through use of the criticality control routine described in section VIII, effects of a control device used to maintain criticality during burnup may also be accounted for.

The burnup calculation involves the solution of a set of differential equations for each region of the reactor. Each of the equations relates the rate of change of concentration of an isotope to its own concentration and to the concentration of its parent isotopes. Thus, if ${}^{k}N_{g}$ is the concentration of the g^{th} isotope present in region k,

$$\frac{d}{dt}\left({}^{k}N_{g}\right) = \sum_{g'} {}^{k}N_{g'}\left[\sum_{i} \frac{{}^{k}\phi^{i}}{k_V} f_{g'} {}^{k}\sigma^{i}_{g'\to g}(E_i - E_{i+1}) \times 10^{-24} + \lambda_{g'\to g}\right] - {}^{k}N_{g}\left[\sum_{i} {}^{k}\sigma^{i}_{a_g} f_g \frac{{}^{k}\phi^{i}}{k_V}(E_i - E_{i+1}) \times 10^{-24} + \lambda_g\right] \quad . \tag{46}$$

Here, f'_g = self-shielding factor for isotope g', and $\sigma_{g'\to g}$ = cross section for production of isotope g from isotope g' . The sets of differential equations are solved by means of a method due to Adams so that, after the first four burnup steps on a material, an estimate of the precision is available. This estimate for each isotope in a region is compared with a pair of tolerance limits, ϵ_4 and ϵ_5, to determine whether Δt should be increased, decreased, or left unchanged.

B. Solution of the Differential Equation

Calculations of the concentrations are made, using estimates of the first through fourth derivatives obtained from the differences of values of the previous first derivatives. Thus, predictions are made with $N^{\rho} = N^{\rho-1} + \Delta t \sum_{i=0}^{3} a_i (\nabla^i \dot{N})^{\rho-1}$, and

$$a_0 = 1,\ a_1 = \frac{1}{2},\ a_2 = \frac{5}{12},\ a_3 = \frac{3}{8} \quad , \tag{47}$$

using the backward differences

$$(\nabla^0 Y)^{\rho} = Y^{\rho} \quad ,$$

$$(\nabla^1 Y)^{\rho} = Y^{\rho} - Y^{\rho-1} \quad , \tag{48a}$$

$$(\nabla^2 Y)^\rho = \nabla^1 Y^\rho - \nabla^1 Y^{\rho-1} = Y^\rho - 2Y^{\rho-1} + Y^{\rho-2} \quad ,$$

$$(\nabla^i Y)^\rho = \nabla^{i-1} Y^\rho - \nabla^{i-1} Y^{\rho-1} = Y^\rho - 3Y^{\rho-1} + 3Y^{\rho-2} - Y^{\rho-3} \quad . \tag{48b}$$

In 48ab the superscript ρ indicates the time at which the concentrations and their rates of change apply. The term N^ρ is the concentration at time t^ρ estimated from data available at time $t^\rho - \Delta t \equiv t^{\rho-1}$. The data available at this time is the concentration, $N^{\rho-1}$; the rate of change at $t^{\rho-1}$, $\dot{N}^{\rho-1}$; and the higher order differences of $\dot{N}$, $(\nabla^i \dot{N})^{\rho-1}$ $(i = 1, 2, 3)$ which yield information of the second through fourth derivatives of N in recent time steps. The 0^{th} order difference, $(\nabla^0 \dot{N})^{\rho-1} \equiv N^{\rho-1}$, is obtained from (46) using the fluxes and concentrations at $t^{\rho-1}$. The fluxes used for this purpose depend, of course, on the properties of all regions, in addition to the one currently being solved.

The value of $\dfrac{\Delta t \nabla^3 \dot{N}}{N^*}$ (where N^* is either N or 1.7×10^{-5}, whichever is larger) is used as a measure of whether the time interval, Δt, is satisfactory. If $\left| \dfrac{\Delta t \nabla^3 N}{N^*} \right| > \epsilon_5$, this is an indication either 1) that changes in concentration of other isotopes in the same region or higher terms in the expansion of the rate of depletion of the isotope in question lead to a requirement for a shorter time step, or 2) that indirect effects of changes in other regions are causing errors.

C. Changing the Time Interval

$$\text{If} \quad \left| \frac{\Delta t \nabla^3 \dot{N}}{N^*} \right| < \epsilon_4 \tag{49}$$

for all isotopes in the reactor, then Δt will be increased by a factor of two for the next step.

$$\text{If} \quad \left| \frac{\Delta t \nabla^3 \dot{N}}{N^*} \right| > \epsilon_5 \quad ; \qquad \epsilon_5 = 20\, \epsilon_4 \tag{50}$$

for any isotope in the reactor, then Δt will be decreased by a factor of two before the new concentrations are computed.

When Δt is decreased, backward differences, ∇^i, corresponding to the new time interval are required for the prediction. These are computed from

$$\begin{pmatrix} \nabla^0 \dot{N} \\ \nabla^1 \dot{N} \\ \nabla^2 \dot{N} \\ \nabla^3 \dot{N} \end{pmatrix}_{new} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/2 & 1/8 & 1/16 \\ 0 & 0 & 1/4 & 1/8 \\ 0 & 0 & 0 & 1/8 \end{pmatrix} \begin{pmatrix} \nabla^0 \dot{N} \\ \nabla^1 \dot{N} \\ \nabla^2 \dot{N} \\ \nabla^3 \dot{N} \end{pmatrix}_{old} ; \quad (51)$$

and the new concentrations are computed by equation 47.

If four backward differences are available, if Δt is less than a maximum permissible value, if Δt was not doubled on the previous time step, and if equation 49 is satisfied, Δt is increased by a factor of two. The new backward differences are computed from

$$\begin{pmatrix} \nabla^0 \dot{N} \\ \nabla^1 \dot{N} \\ \nabla^2 \dot{N} \\ \nabla^3 \dot{N} \end{pmatrix}_{new} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 4 & -4 \\ 0 & 0 & 0 & 8 \end{pmatrix} \begin{pmatrix} \nabla^0 \dot{N} \\ \nabla^1 \dot{N} \\ \nabla^2 \dot{N} \\ \nabla^3 \dot{N} \end{pmatrix}_{old} . \quad (52)$$

D. Matrix Elements

The calculation of the right hand side of (46) is essentially a matter of collecting the pertinent cross sections. Most of the terms are zero; that is, only a small number of the isotopes present in region k contribute to the production of any particular isotope in that region. On the group cross section tape and on the basic library along with the cross section data for each isotope are the following data:

- A - isotope name
- a_A - atomic weight of A
- A'_{0A} - name of isotope produced when a neutron is captured by an A atom
- A'_{1A} - name of an isotope produced when a neutron causes fission of an A atom
- Y_{1A} - yield of A'_{1A} in fission of A
- A'_{2A} - name of another fission product of A
- Y_{2A} - yield of A'_{2A} in fission of A

- (up to 9 fission products per isotope)

λ - total radioactive decay constant for isotope A in reciprocal seconds

$A'_{d_1 A}$ - name of an isotope produced by radioactive decay of an A atom

λ'_{1A} - radioactive decay constant for A in chain producing $A'_{d_1 A}$

$A'_{d_2 A}$ - name of another decay product of A

λ_{2A} - decay constant for A for production of $A'_{d_2 A}$

- (up to 3 decay products for each isotope)

This information governs the selection of cross sections for the $\sigma_{g \rightarrow g'}$ from the σ_{c_A} and σ_{f_A}. The number of fission products and decay products may vary from isotope to isotope.

VII. THE ADJOINT EQUATION

At the computer's option, DMM may be used to calculate the adjoint fluxes. The equation adjoint to equation 1 is

$$\nabla [D(r, E) \nabla \phi^{*} (r,E)] - \Sigma_{t} (r,E) \phi^{*} (r,E)$$

$$+ \sum_{A} \Sigma_{in_A} (r,E) \frac{\nu_{in_A} (r,E)}{X_{in_A} (r,E)} \int_{E_{min}}^{E} \chi_{in_A} (r,E') \phi^{*} (r,E') dE'$$

$$+ \sum_{A} \frac{\Sigma_{s_A} (E)}{(1-\alpha_A) E} \int_{\max(E_{min}, \alpha_A E)}^{E} \phi^{*} (r,E') dE'$$

$$= \frac{1}{k^{*}} \Sigma_{f} (r,E) \nu_{f} (r,E) \int_{E_{min}}^{E_{max}} \chi_{f} (r,E') \phi^{*} (r,E') dE' \quad . \tag{53}$$

The corresponding multigroup equations are almost identical in form to equations 3, 4, and 5.

$$- \nabla [D^{*i} (r) \nabla \phi^{*i} (r)] + T^{*i} (r) \phi^{*i} (r) = H^{*i} (r) \quad i = 1, 2, 3 \ldots I.$$

$$H^{*i} (r) = \sum_{j=i+1}^{I} T^{*ij} (r) \phi^{*j} (r) + \chi_{f}^{*i} P^{*} (r) \quad .$$

$$P^{*} (r) = \frac{1}{k} \sum_{j=1}^{I} F^{*j} (r) \phi^{*j} (r) \quad . \tag{54}$$

The only difference between these equations and equations 3, 4, and 5 is that the sum in equation 54 is over $j > i$, while in equation 4 it is over $j < i$. The definitions of some of the nuclear constants, however, are quite different. The adjoint equations analogous to equations 20 through 25 are

$$D^{*i} \equiv \frac{1}{3} \left\{ \left[\int_{E_{i+1}}^{E_i} \Sigma_{tr} (E) \phi^{*} (E) dE \right] \Big/ \phi^{*i} (E_i - E_{i+1}) \right\}^{-1} \quad . \tag{55}$$

$$T^{*i} \equiv \left[\int_{E_{i+1}}^{E_i} \left\{ \Sigma_t(E)\phi(E) - \sum_A \Sigma_{in_A}(E) \; X_{in_A}(E) \int_{E_{i+1}}^{E} \chi_{in_A}(E')\,\phi^*(E')\,dE' \right.\right.$$

$$\left.\left. - \sum_A \frac{\Sigma_{s_A}(E)}{(1-\alpha_A)E} \int_{\max(E_{i+1}, \alpha_A E)}^{E} \phi^*(E')\,dE' \right\} dE \right] \Bigg/ \phi^{*i}(E_i - E_{i+1})$$

$$+ [B^2 D]^i \quad . \tag{56}$$

$$T^{*ij} \equiv \left[\int_{E_{i+1}}^{E_i} \left\{ \sum_A \frac{\Sigma_{in_A}(E)\,\nu_{in_A}(E)}{X_{in_A}(E)} \int_{E_{j+1}}^{E_j} \chi_{in_A}(E')\phi^*(E')\,dE' \right.\right.$$

$$\left.\left. + \sum_A \frac{\Sigma_{s_A}(E)}{(1-\alpha_A)E} \int_{\max(E_{j+1}, \alpha_A E)}^{E_j} \phi^*(E')\,dE' \right\} dE \right] \Bigg/ \phi^{*j}(E_i - E_{i+1}) \text{ if } j > i. \tag{57}$$

$$T^{*ij} = 0 \text{ if } j \leq i \quad .$$

$$\chi_f^{*i} \equiv \left[\int_{E_{i+1}}^{E_i} \Sigma_f(E)\nu_f(E)\,dE \right] \Bigg/ (E_i - E_{i+1}) \quad . \tag{58}$$

$$F^{*j} \equiv \left[\int_{E_{j+1}}^{E_j} \chi_f(E)\phi^*(E)\,dE \right] \Bigg/ \phi^{*j} \quad . \tag{59}$$

$$\Sigma_f^{*j} = \left[\int_{E_{j+1}}^{E_j} \chi_f(E)\, \phi^*(E)\, dE \right] \Big/ \phi^{*j} \tag{59a}$$

$$\phi^{*i} \equiv \int_{E_{i+1}}^{E_i} \phi^*(E)\, dE \Big/ (E_i - E_{i+1}) \quad . \tag{60}$$

In DMM, flux weighting is not included in the adjoint cross section calculations. As a result, renaming the groups and the fission constants provides a formal identity between the adjoint and normal calculations. To carry this out, one must return to the input routine and re-evaluate the nuclear constants with no flux weighting, or carry out the adjoint calculation before the normal diffusion calculation is carried out.

VIII. CRITICALITY CONTROL

The criticality subroutine of DMM is used in order to determine critical conditions and to maintain criticality by simulating the motion of a control rod during the burnup calculation. When used to determine critical conditions, it may be applied in conjunction with either the straight multigroup diffusion or the adjoint calculations. Its use during burnup calculations is required to maintain the spectrum appropriate to actual reactor operation and to assure the proper normalization of the fluxes. As input, it is necessary to specify the address of a single quantity Z that is to be varied, a first guess (δ) for the reciprocal of the derivative of $\mathcal{k}$ with respect to Z, the reactivity desired ($\mathcal{k}_0$), and the tolerance (ϵ_3) for the deviation of the final reactivity from $\mathcal{k}_0$. The parameter to be varied might be, for example, the mesh spacing in any region, the concentration of one component in any region, or the transverse leakage.

If $(\mathcal{k}_0 - \mathcal{k}_i) > \epsilon_3$, a new trial value of Z is computed from

$$Z_{i+1} = Z_i + \delta\,(\mathcal{k}_0 - \mathcal{k}_i) \quad . \tag{61}$$

When $\mathcal{k}_{i+1}$ has been determined, δ is replaced by

$$\delta = \frac{Z_{i+1} - Z_i}{\mathcal{k}_{i+1} - \mathcal{k}_i} \quad . \tag{62}$$

However, when three successive Z_i have been computed by (61), instead of using the third of these, the program replaces the third one by

$$Z'_{i+1} = Z_{i+1} - \frac{(Z_{i+1} - Z_i)^2}{(Z_{i+1} - 2Z_i + Z_{i-1})} \quad , \tag{63}$$

thus using Aitken's δ^2 method to extrapolate to a better estimate of the critical value of Z.

Each time equation 63 is used and each time a Z is found such that $(\mathcal{k}_0 - \mathcal{k}_i) \leq \epsilon_3$, the program must begin once more accumulating a set of three Z_i before (63) may be used again.

IX. NEUTRON BALANCE

DMM can compute the various components of neutron transfer from and to each group and region and print these out. The quantities calculated for each group and region are:

1. The total neutron flux per unit energy in group i of region k:

$$ {}^{k}\phi^{i} = \phi^{i}_{N_{k-1}} \Delta V_{N^{+}_{k-1}} + \sum_{N_{k-1}+1}^{N_k - 1} \phi^{i}_{n} \Delta V_{n} + \phi^{i}_{N_k} \Delta V_{N^{-}_{k}} . $$

2. The total fission neutron source in region k:*

$$ {}^{k}P = P_{N^{+}_{k-1}} \Delta V_{N^{+}_{k-1}} + \sum_{N_{k-1}+1}^{N_k - 1} P_{n} \Delta V_{n} + P_{N^{-}_{k}} \Delta V_{N^{-}_{k}} . $$

3. The degradation from group i in region k to lower energy groups:

$$ {}^{k}\mathcal{D}^{i} = {}^{k}\phi^{i} \sum_{j=i+1}^{I} {}^{k}T^{ji} \left(\frac{E_j - E_{j+1}}{E_i - E_{i+1}} \right) . $$

4. The scattering from higher energy groups into group i of region k:

$$ {}^{k}S^{i} = \sum_{j=1}^{i-1} {}^{k}T^{ij} \, {}^{k}\phi^{j} . $$

5. The fission neutron source in group i of region k:

$$ {}^{k}\mathcal{F}^{i} = \chi^{i}_{f} \, {}^{k}P . $$

6. The removal from group i of region k due to perpendicular leakage:

$$ {}^{k}L^{i}_{P} = {}^{k}(B^2 D)^{i} \, {}^{k}\phi^{i} . $$

7. The removal due to absorption from group i of region k:

$$ {}^{k}C^{i} = ({}^{k}T^{i} \, {}^{k}\phi^{i}) - {}^{k}\mathcal{D}^{i} - {}^{k}L^{i}_{P} . $$

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* This is the portion of the normalized source $1/\lambda\, F\phi$ that is produced in region k_j; although it is the source which produces the ${}^{k}\phi^{i}$, it is not really that which would be produced by them unless $\lambda = 1$. The possibility of a difference between the source that produces a set of fluxes and the source resulting from those fluxes is one reason for the necessity of maintaining criticality during burnup calculations.

8. The removal due to leakage from the outer boundary of region k in group i:

$$k_{L_+}^{i} = - k_D^{i} \frac{\phi_{N_k}^{i} - \phi_{N_k-1}^{i}}{k_{\Delta r}} .$$

9. The removal due to leakage from the inner boundary of region k in group i:

$$k_{L_-}^{i} = k_D^{i} \frac{\phi_{N_{k-1}+1}^{i} - \phi_{N_{k-1}}^{i}}{k_{\Delta r}} .$$

10. The total removal from group i of region k:

$$k_R^{i} = k_C^{i} + k_{\mathcal{D}}^{i} + k_{L_P}^{i} + k_{L_+}^{i} + k_{L_-}^{i} .$$

11. The total production in group i of region k:

$$k_P^{i} = k_S^{i} + k_{\mathcal{F}}^{i} .$$

12. The total leakage in region k:

$$k_L = \sum_{i=1}^{I} \left(k_{L_+}^{i} + k_{L_-}^{i} \right) + k_{L_P}^{i} .$$

13. The error in neutron balance for region k:

$$k_{\mathcal{E}} = \left| \frac{\sum_{i=1}^{I} \left(k_P^{i} - k_R^{i} \right)}{\sum_{i=1}^{I} k_P^{i}} \right| .$$

14. The fission neutron product from group i of region k:

$$k_{\bar{F}}^{i} = k_F^{i} \; k_{\phi}^{i} .$$

X. FLOW CHARTS

A. Basic Library Preparation

B. Problem Input

C. Monitor

D. Diffusion Calculation

E. Microscopic Group Tape Preparation

F. Macroscopic Constants

G. Burnup Constants

H. Adjoint Modification

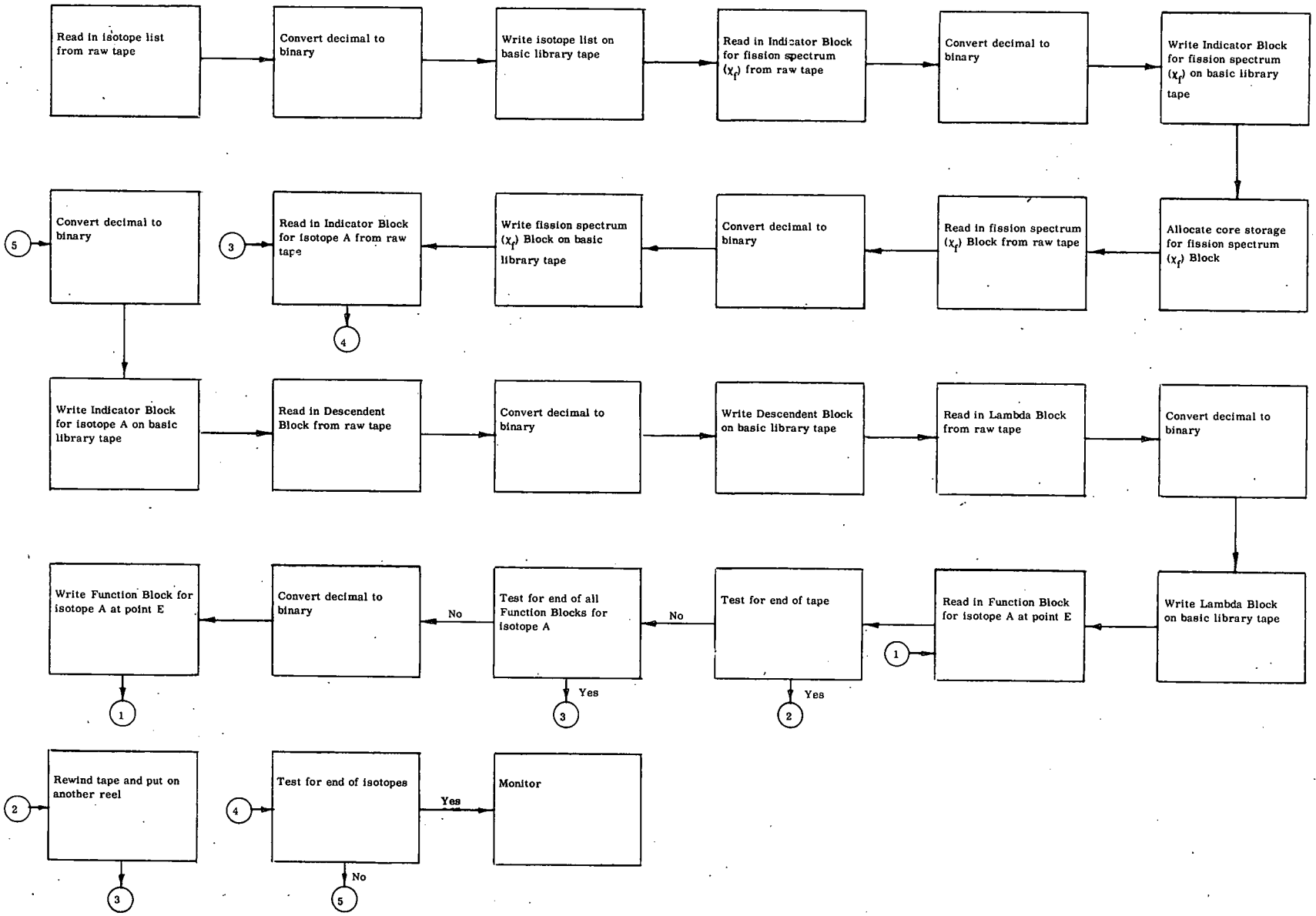
I. Determination of Critical Conditions

J. Neutron Balance

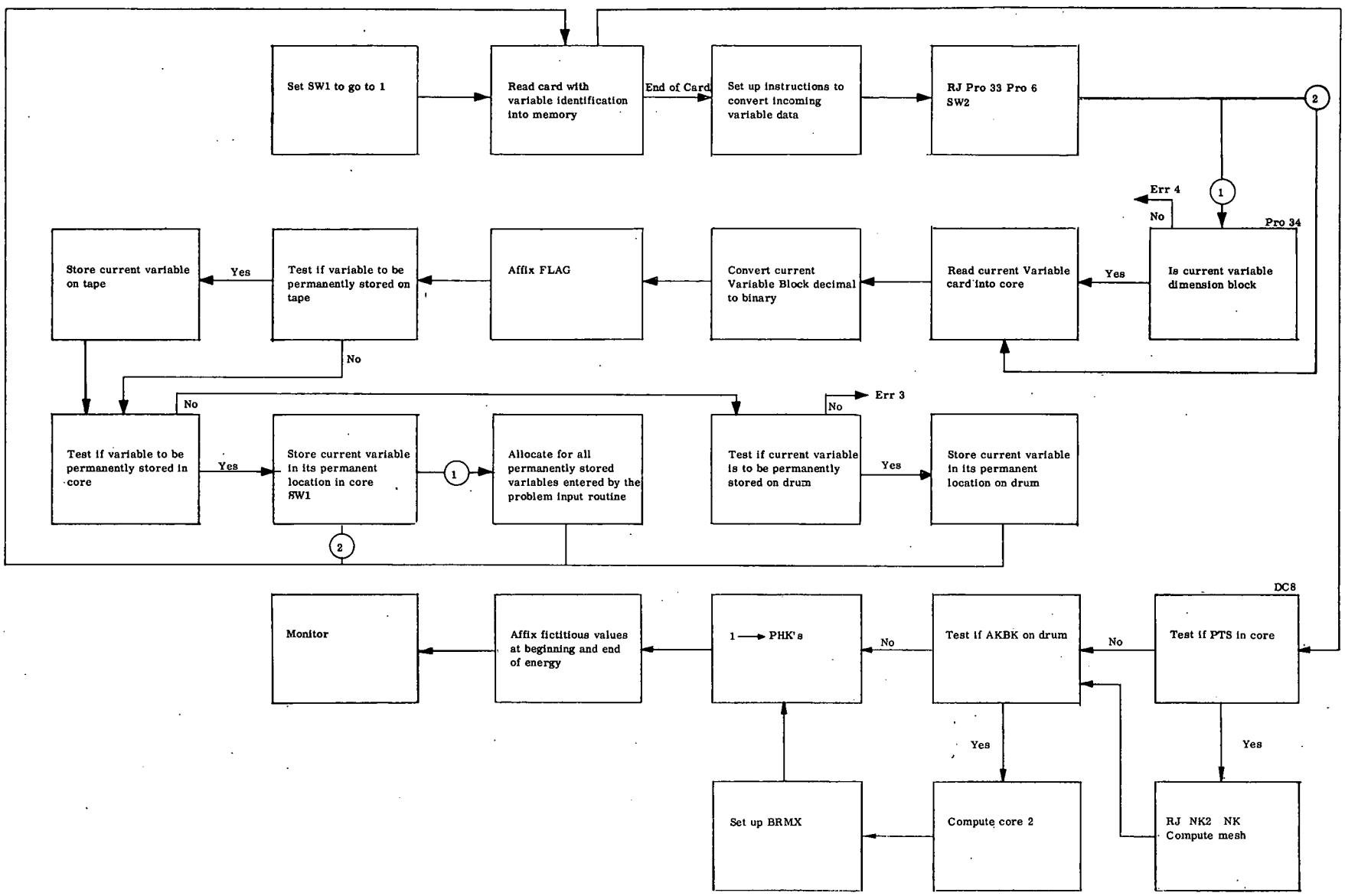
K. Xenon and Samarium Addition

L. Output

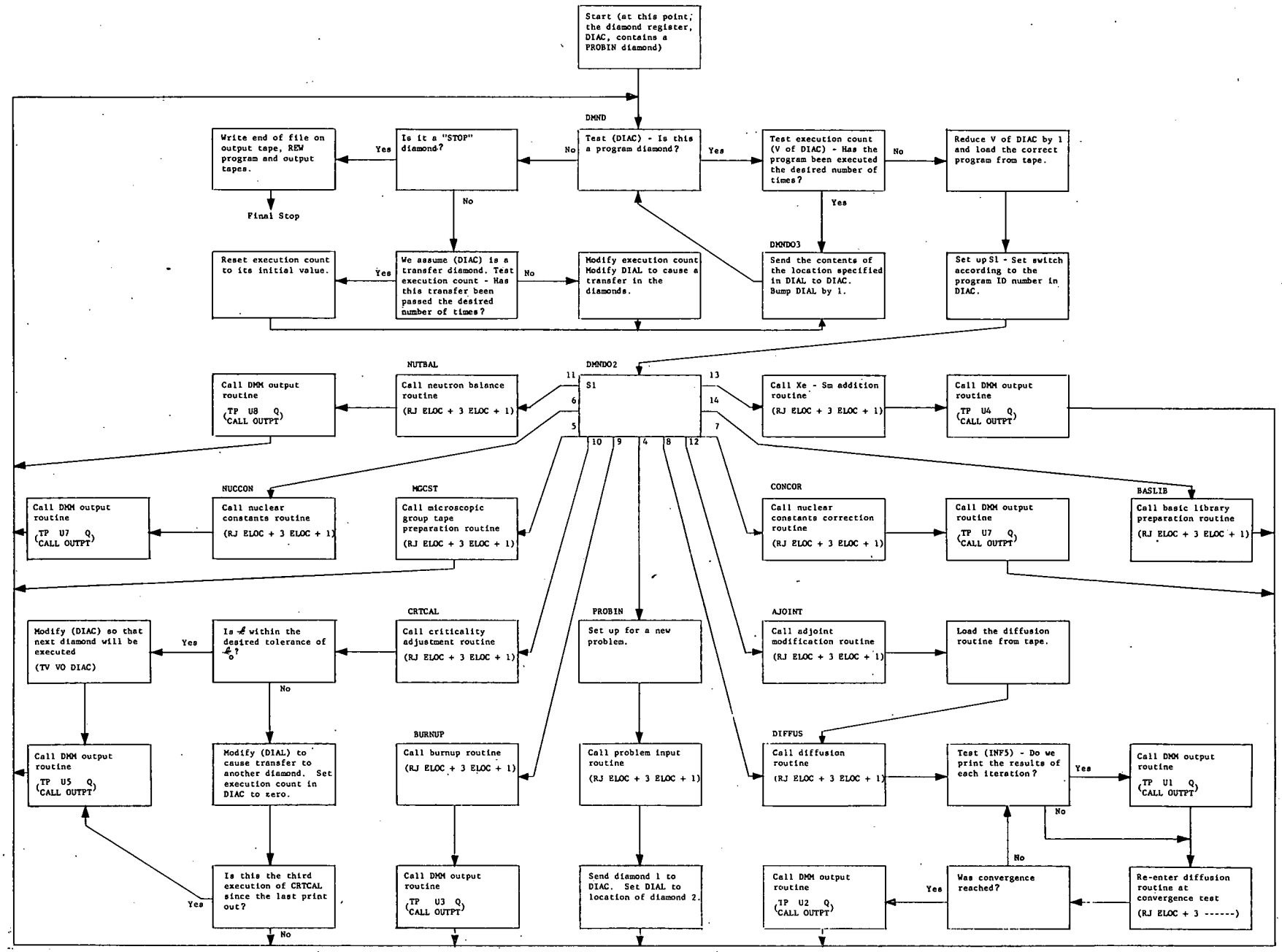
A. BASIC LIBRARY PREPARATION



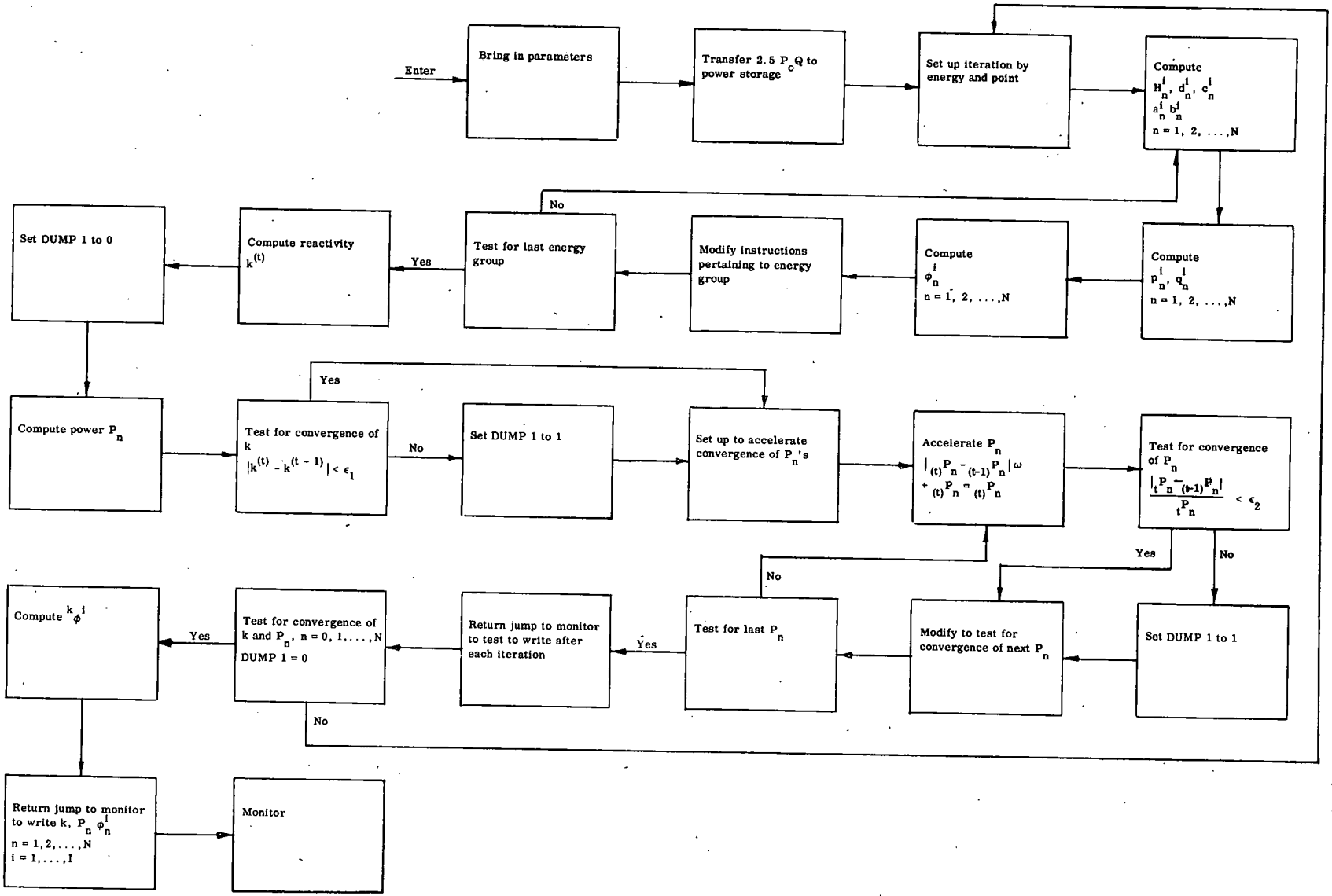
B. PROBLEM INPUT



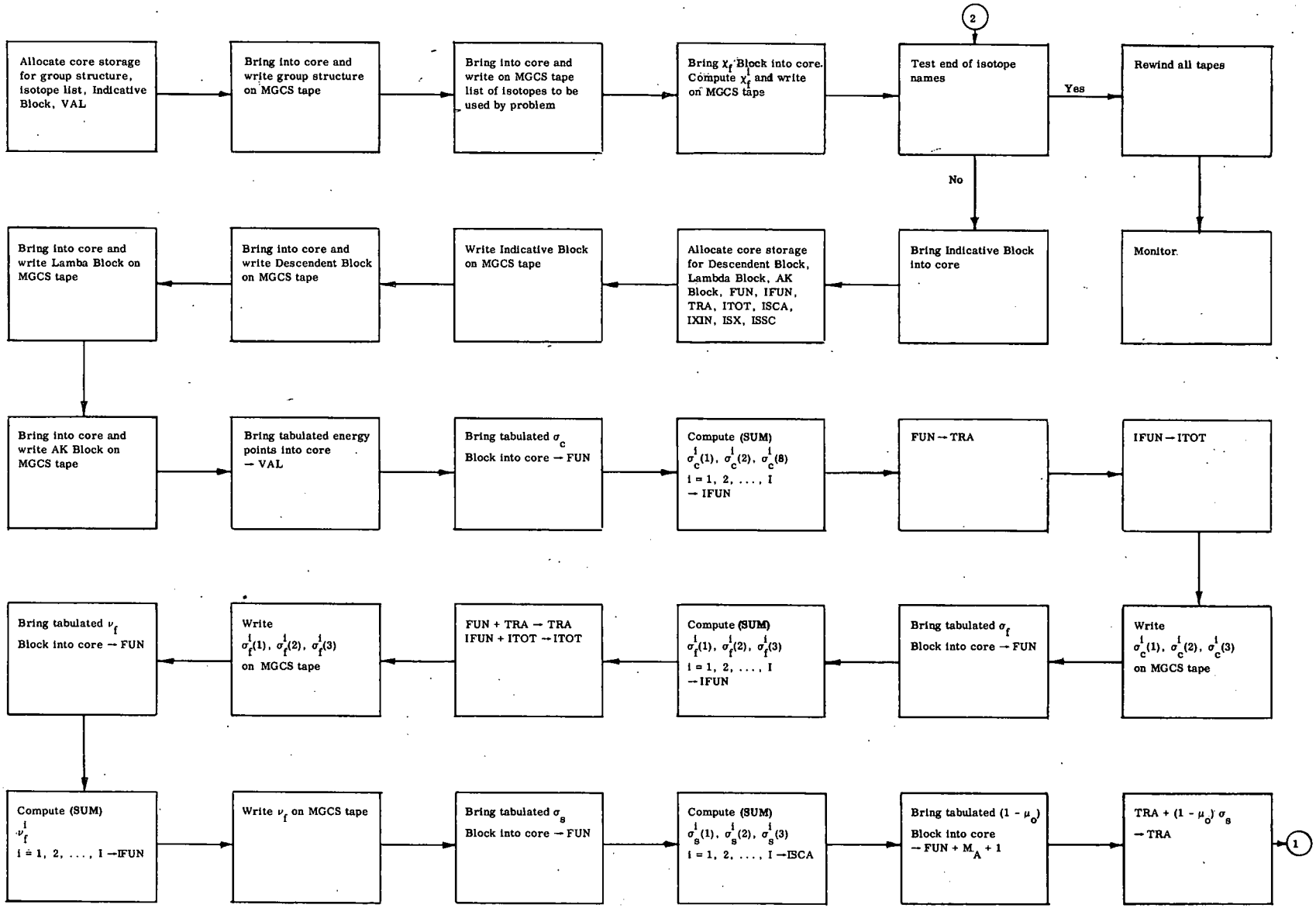
C. MONITOR


Start (at this point, the diamond register, DIAC, contains a PROBIN diamond)
DMND
Test (DIAC) - Is this a program diamond?
No
Yes
Is it a "STOP" diamond?
Yes
Write end of file on output tape, REW program and output tapes.
Final Stop
No
Test execution count (V of DIAC) - Has the program been executed the desired number of times?
Yes
No
Reduce V of DIAC by 1 and load the correct program from tape.
DMNDO3
Send the contents of the location specified in DIAL to DIAC. Bump DIAL by 1.
Modify execution count Modify DIAL to cause a transfer in the diamonds.
We assume (DIAC) is a transfer diamond. Test execution count - Has this transfer been passed the desired number of times?
Yes
No
Reset execution count to its initial value.
Set up S1 - Set switch according to the program ID number in DIAC.
DMNDO2
S1
11
6
5
13
14
7
10
9
4
8
12
NUTBAL
Call neutron balance routine
(RJ ELOC + 3 ELOC + 1)
Call DMM output routine
(TP U8 Q CALL OUTPT)
Call Xe - Sm addition routine
(RJ ELOC + 3 ELOC + 1)
Call DMM output routine
(TP U4 Q CALL OUTPT)
NUCCON
Call nuclear constants routine
(RJ ELOC + 3 ELOC + 1)
Call DMM output routine
(TP U7 Q CALL OUTPT)
MGCST
Call microscopic group tape preparation routine
(RJ ELOC + 3 ELOC + 1)
CONCOR
Call nuclear constants correction routine
(RJ ELOC + 3 ELOC + 1)
Call DMM output routine
(TP U7 Q CALL OUTPT)
BASLIB
Call basic library preparation routine
(RJ ELOC + 3 ELOC + 1)
CRTCAL
Call criticality adjustment routine
(RJ ELOC + 3 ELOC + 1)
Is δ within the desired tolerance of δ0?
Yes
No
Modify (DIAC) so that next diamond will be executed
(TV VO DIAC)
PROBIN
Set up for a new problem.
AJOINT
Call adjoint modification routine
(RJ ELOC + 3 ELOC + 1)
Load the diffusion routine from tape.
BURNUP
Call burnup routine
(RJ ELOC + 3 ELOC + 1)
Modify (DIAL) to cause transfer to another diamond. Set execution count in DIAC to zero.
Call DMM output routine
(TP U5 Q CALL OUTPT)
Call problem input routine
(RJ ELOC + 3 ELOC + 1)
DIFFUS
Call diffusion routine
(RJ ELOC + 3 ELOC + 1)
Test (INF5) - Do we print the results of each iteration?
Yes
No
Call DMM output routine
(TP U1 Q CALL OUTPT)
Is this the third execution of CRTCAL since the last print out?
Yes
No
Call DMM output routine
(TP U3 Q CALL OUTPT)
Send diamond 1 to DIAC. Set DIAL to location of diamond 2.
Call DMM output routine
(TP U2 Q CALL OUTPT)
Yes
Was convergence reached?
No
Re-enter diffusion routine at convergence test
(RJ ELOC + 3 ------)

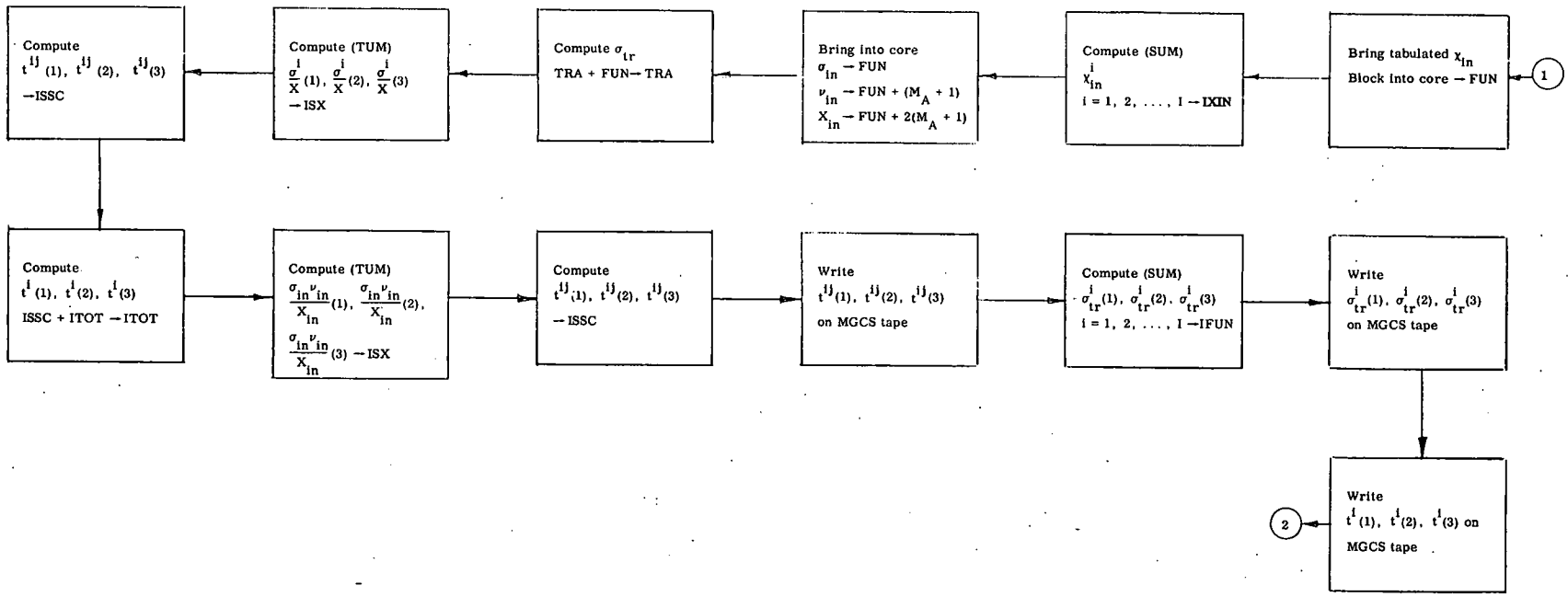
D. DIFFUSION CALCULATION



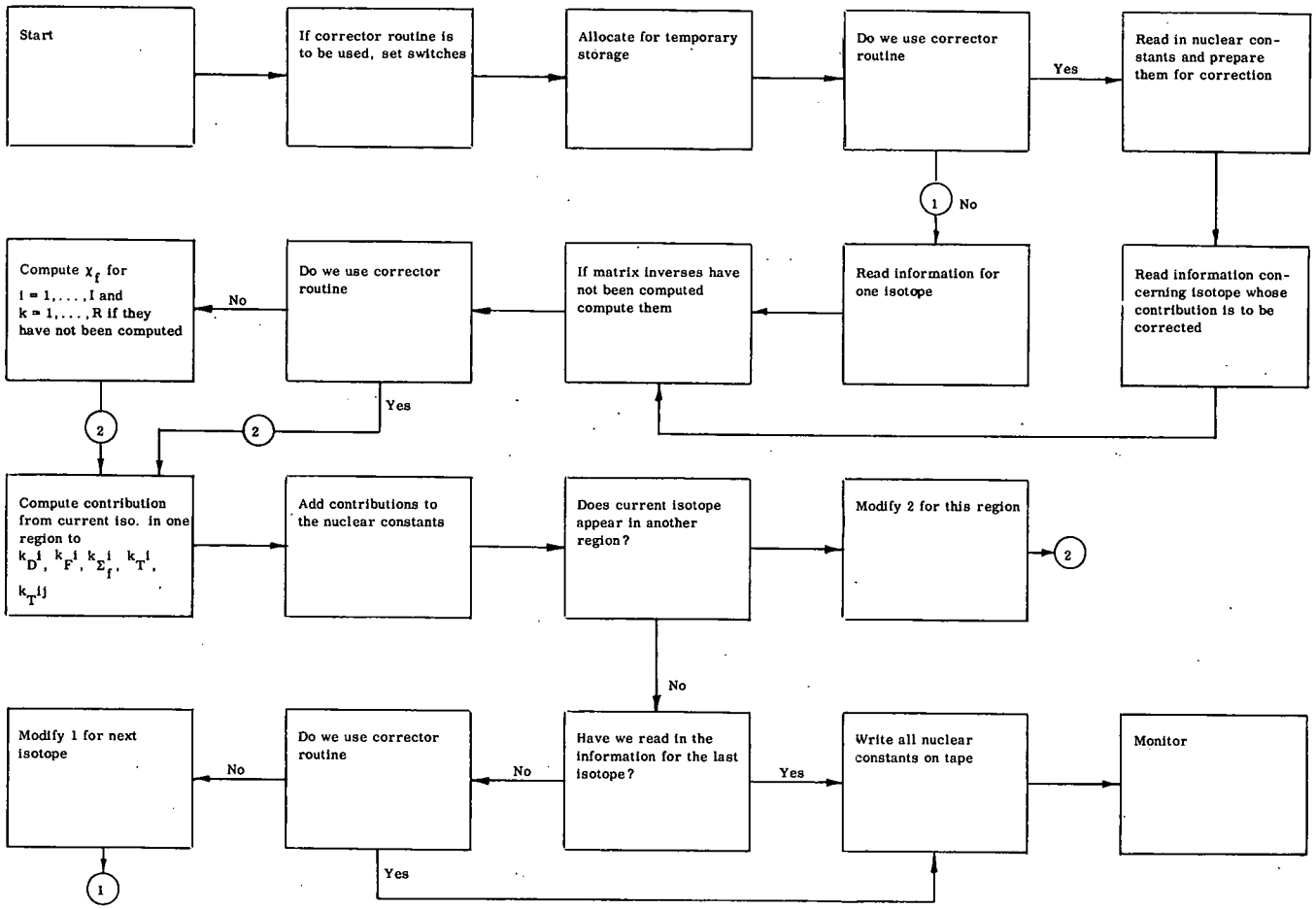
E. MICROSCOPIC GROUP TAPE PREPARATION



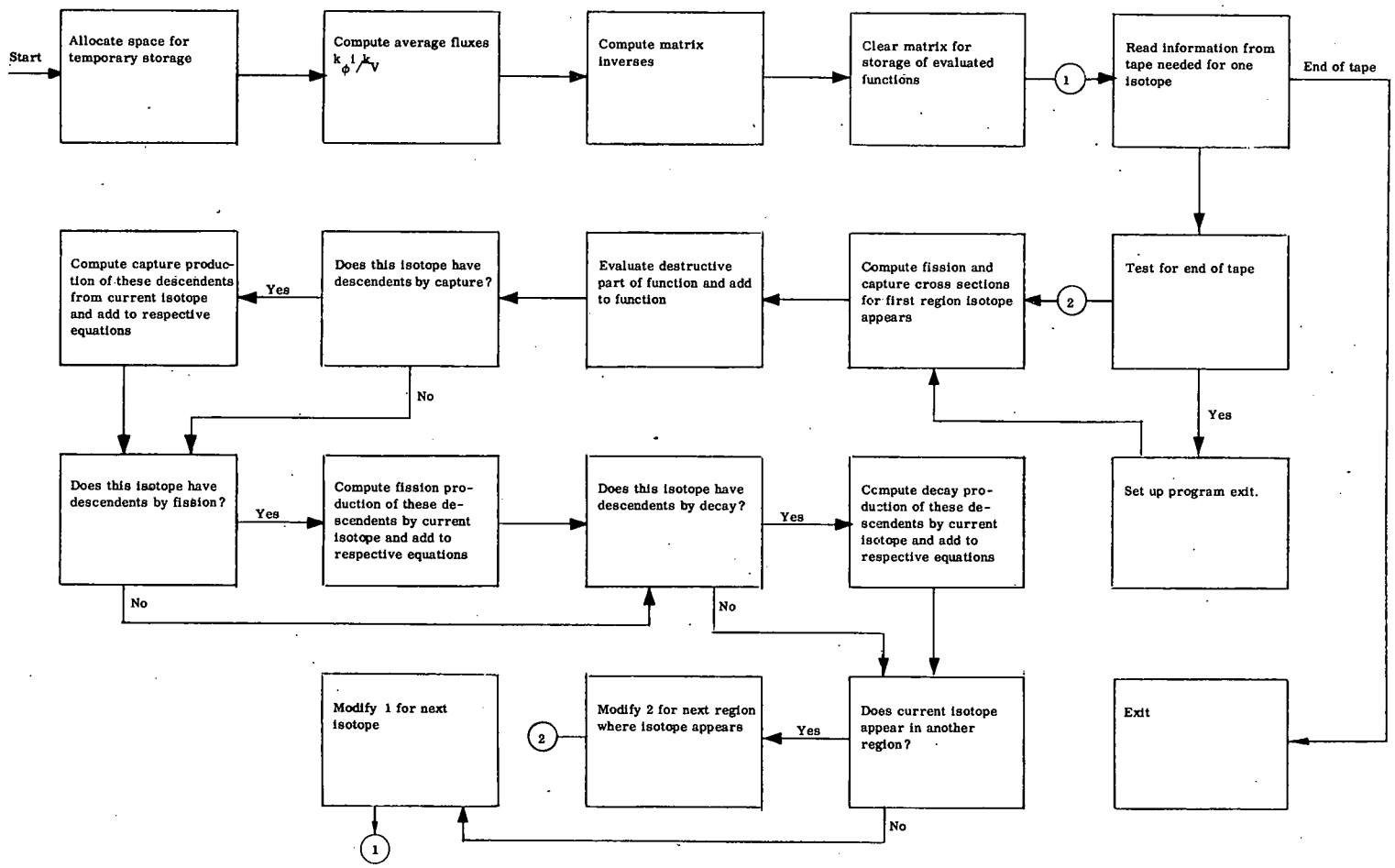
E. MICROSCOPIC GROUP TAPE PREPARATION
(Page 2)



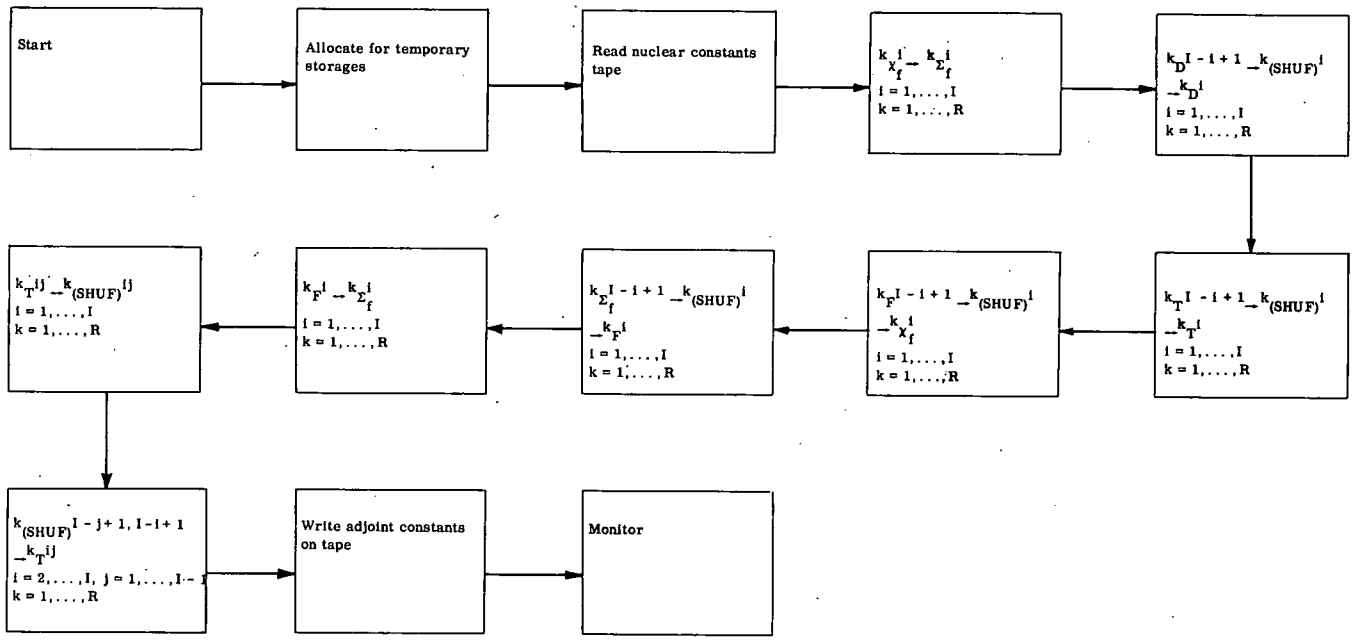
F. MACROSCOPIC CONSTANTS



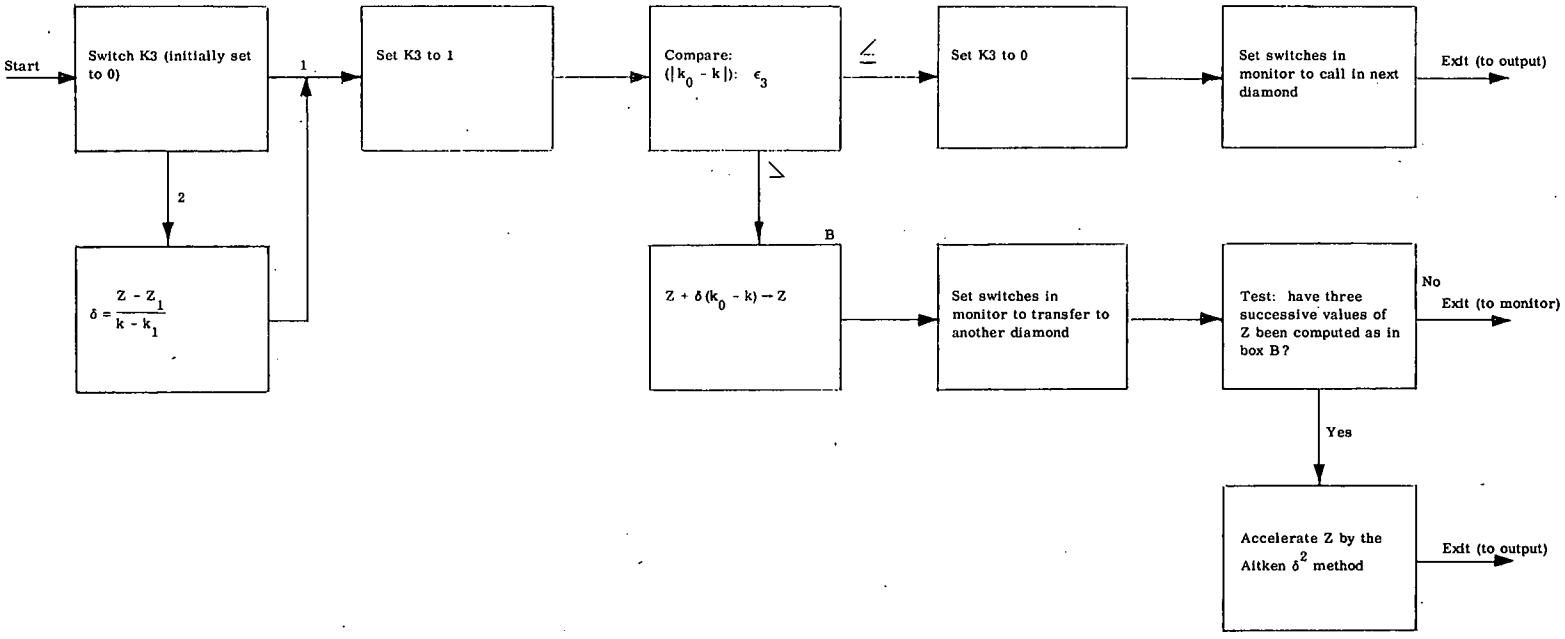
G. BURNUP CONSTANTS



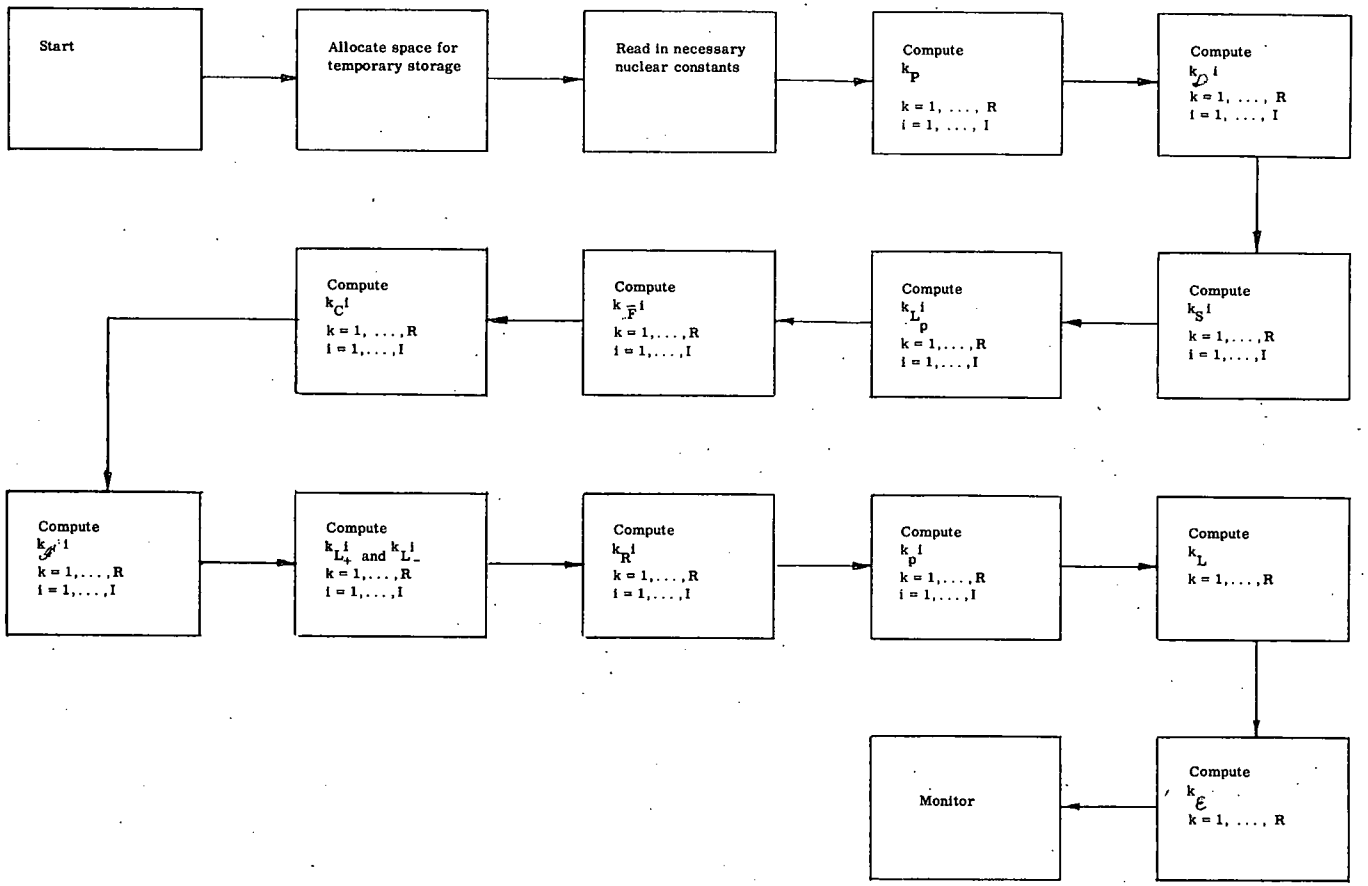
H. ADJOINT MODIFICATION



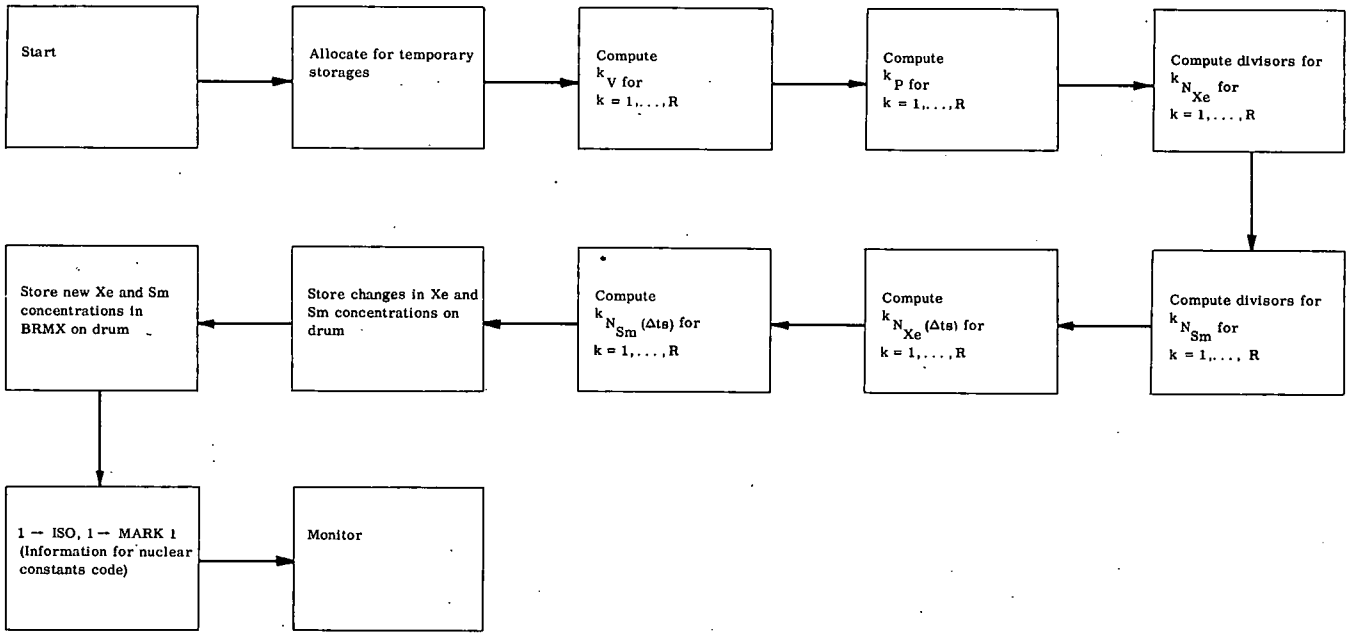
I. DETERMINATION OF CRITICAL CONDITIONS



J. NEUTRON BALANCE



K. XENON AND SAMARIUM ADDITION



L. PROBLEM OUTPUT