A S T U D Y O F T H E T W O D I M E N S I O N A L M U L T I G R O U P D I F F U S I O N A N A L Y S I S C O D E: E R E B U S

by

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ÖZET

Bu çalışmanın amacı EREBUS isimli, çok guruplu difuzyon denklemini iki boyutlu geometride çözerek kritikalite araştırması yapan bilgisayar programını detayıyla incelemektir. EREBUS EURATOM, FIAT ve ARS'nin yardımıyla M. Console, A. Daneri ve E. Salina tarafından geliştirilmiş olup Boğaziçi Üniversitesindeki UNIVAC 1106 sistemine uygulanmıştır. Programın dili FORTRAN IV'dür.

Bu bilgisayar programı difüzyon denklemini iki boyutlu (x-y, r-z veya r-θ) geometride sonlu farklar yöntemiyle diskritize ederek çözmekte ve gerekli olan mikroskopik tesir kesitleri değişik bilgisayar programları tarafından hazırlanabilmektedir. Fakat, GKSS'nin (Gessellschaft für Kernenergieverwertung in Schiffbau und Schiffahrt mbH.) yardımıyla K. Pendorf, F. Schult, ve G. Schulz tarafından geliştirilmiş olan GELS kodu bu amaç için en uygunudur.

EREBUS bir ana program ve muhtelif alt programlar içerir. Bunların yaptıkları işler aşağıdaki şekilde sıralanabilir.

1. Giriş bilgilerinin okunması, kontrol edilmesi, düzenlenmesi ve yazılması.

2. Gurup sabitlerinin ve makroskopik tesir kesitlerinin hesaplanması.

3. Difüzyon denkleminin sonlu farklar yöntemiyle diskritize edilmesi ve katsayıların hesaplanması.

4. Sonlu fark denklemlerinin çözümü.

5. Yakıt elemanlarındaki yanma miktarlarının ve fizyon ürünlerinin belirlenen zaman dilimlerinde hesaplanması.

6. Elde edilen bilgilerin düzenlenerek yazılması.

ABSTRACT

The purpose of this study is to examine and explain [illegible] computer code CERBUS. It is a multi-group diffusion [illegible] code in two dimensions, with criticality searches. This code has been developed by M. Consolo, A. Donori, and M. Settimo under the auspices of NURATOM-FIAT-ANS and is adapted to the I.B.M. 1620 system at BOĞAZİÇİ UNIVERSITY. Program language is CERBUS II and FORTRAN IV.

CERBUS is designed to solve problems involving the finite difference representation of the diffusion theory has been [illegible] to two space dimensions in either x-y or r-z geometry.

The microscopic cross section data for this code is [illegible] generated by various codes but, GRUF, developed by K. Rehm[illegible], Schmidt of K. Schulz under the auspices of GRS (Gesellschaft für Kernverfahrenstechnik in Schiffbau und Schiffahrt m.b.H.) is designed specifically for this purpose.

CERBUS consists of one main program and several subprograms the major sections of which perform the following functions:

1. Processing of the input data, including checking, and printing.

2. Calculation of the required macroscopic cross sections and group parameters.

3. Calculation of the coefficients for the finite difference [illegible] used to approximate the group diffusion [illegible] with the interface and [illegible] boundary conditions.

4. Solution of the eigenvalue problem represented by the finite difference equations.

5. [illegible] calculation of the fuel depletion and accumulation of fission products for a specified time step.

6. Printing of the selective information for [illegible] and punching.

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NOMENCLATURE

SYMBOL		CHARACTERIZE
WABS(J)	:	Absorption term for the J^{th} isotope
XX	:	Actual power density
A(J)	:	Atomic weight of the J^{th} isotope
Av	:	Avogadro Number
J	:	Burnable (time dependent) isotope index
M	:	Composition index
	:	Decay constant
O	:	Dilution factor
VOLEA	:	Effective volume of the reactor
FSENT	:	Fission source term
YIELD	:	Fission yield
XFASS	:	Form factor
YASS	:	Integrated actual power
QPSOR	:	Integrated actual source
PP	:	Integrated actual volume flux
ABSNT	:	Losses due to absorption, removal and transversal leakage
Σ_a	:	Macroscopic absorption cross section
Σ_r	:	Macroscopic cross section for energy production
Σ_f	:	Macroscopic fission cross section
Σ_r	:	Macroscopic removal cross section
N(L)	:	Number density in region L
Φ	:	Neutron flux
L	:	Region index

SCSOR	:	Scattering collision source
	:	Self-Shielding factor
$W(J)$	:	Total weight of the J^{th} burnable isotope in reactor
$W(M,J)$	:	Weight of the J^{th} burnable isotope in composition M
$W(L,J)$	:	Weight of the J^{th} burnable isotope in region L

CHAPTER I

INTRODUCTION

The purpose of this study is to examine and explain the [illegible] pulse program KENDUS which is a multigroup diffusion [illegible] dimensions, with criticality searches. This code is [illegible] of Fortran and is the computers of the IBM-360 series [illegible] which have large directly addressable storage. It is [illegible] by H. Conde-le, A. Benard and F. Sallen under the supervision [illegible] ARG in Fortran IV language and has been adapted [illegible] University System at Beijing Universidy.

[illegible] is designed to solve problems involving the [illegible] diffusion approximation of diffusion theory in [illegible] arbitrary with arbitrary finite-group neutron [illegible] which may be solved by using an eigenfunction formulation [illegible] criticality analysis.

[illegible] factor is a device in which numerous [illegible] can be arranged that a self sustained fission [illegible] can occur in a controlled manner. The neutron [illegible] factor, self sustained chain reaction is one [illegible] initially by one of the neutrons produced [illegible] of the reactor in induced another fission. In [illegible] only, the fission must just be sustained, [illegible] of the fission reaction within the system will [illegible] by [illegible] other hand, such fission could [illegible] [illegible], the fission must be kept [illegible] the neutron population constant, [illegible] [illegible] is known as the [illegible] [illegible] and can vary from [illegible] [illegible] fission induced by a single fission of the [illegible] [illegible].

[illegible] can be expressed conveniently in terms [illegible] factor, this is defined as the [illegible] [illegible] a generation to the [illegible] [illegible] mathematically, therefore, there [illegible] [illegible] must be unity for a number of fissile [illegible] [illegible] to a constant rate and such a system [illegible]

critical. If the multiplication factor is greater than unity, a number of fission neutrons with each succeeding generation increases, which means, the chain reaction diverges and the system is said to be supercritical. Finally, if the multiplication factor is less than unity, the chain reaction eventually dies out, and the system is called subcritical.

Energy, space and time dependent neutron diffusion equation describing the balance of competing processes that take place in a multiplying medium can be written as;

$$\nabla\cdot D(r,E)\nabla\phi(r,E,t) - \Sigma_t(r,E)\phi(r,E,t) + \chi(E)\int_0^\infty \nu\Sigma_f(r,E')\phi(r,E',t)dE' = \frac{1}{v(E)}\frac{\partial}{\partial t}\phi(r,E,t) \qquad (1.1)$$

When the system is in a steady state, the time derivative is zero and it could already vanish and the resulting equation would be independent, a critical system. In search for this solution, one can modify the above equation by the introduction of a parameter λ as follows;

$$-\nabla\cdot D(r,E)\nabla\phi(r,E) + \Sigma_t(r,E)\phi(r,E) = \frac{\chi(E)}{\lambda}\int_0^\infty \nu\Sigma_f(r,E')\phi(r,E')dE' \qquad (1.2)$$

In passing from Equation (1.1) to Equation (1.2) the neutron source is divided by λ and the time derivative has been set equal to zero, thereby this mathematical step corresponds to dividing the fission source by a factor $1/\lambda$ so as to bring the system into a critical condition, i.e. critical system is the solution of the [illegible] is described by [illegible] system under investigation [illegible] of λ be so [illegible] the system is [illegible] the value of λ [illegible] the [illegible] equation (1.2) [illegible] symbol [illegible] of the [illegible] solutions [illegible] such as Σ_a [illegible] neutron [illegible] of [illegible] the [illegible] system [illegible] words, we have [illegible] which can maintain a time independent chain [illegible]

system. As will be made clear later in this work this factor is simply the same thing as the multiplication factor in one group theory.

The solution of the energy dependent diffusion equation in two dimensions can be broken down into several stages. In stage one, the multigroup approximation can be developed. In stage two, having the problem can be solved by the source iteration method; this method reduces the solution of the multigroup problem to the solution of a series of one group problems. In stage three we will discuss setting up the finite difference approximation in two dimensional case. In stage four, the solution of the multigroup equations will be discussed.

There are three basic difficulties in the solution of the finite difference equations. Firstly, the equations can not be solved directly, hence an iterative method has to be used. Secondly, very large mesh points of the order of 3000 to 10000 per group, have to be used. Thirdly, the two dimensional problem will usually require the use of magnetic tape or disc storage to solve, with a consequent increase in running time and a decrease in flexibility.

We will now allow the neutron flux to depend on energy, that is rather than treat the neutron energy variable as a continuous variable, we will immediately discretize it into a number of finite energy groups as schematically shown below;

$$E_0 \quad E_1 \quad \cdots \quad E_{g-1} \quad E_g \quad \cdots \quad E_{G-1} \quad E_G$$

$$\text{group } g \qquad \text{group } G$$

Notice that we are using a backward indexing scheme, corresponding to the fact that the neutron energy is decreasing as the lifetime and collisions go by. Also note that the discretized equations above will be indexing successively to lower energies.

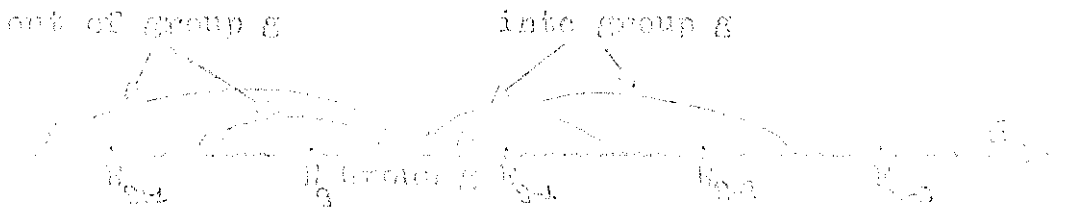
It is now possible to discretize $\phi(\vec{r},E)$ by considering only the flux defined at each energy mesh point E_g, but we must still have to define the discretized flux to be the integral of $\phi(\vec{r},E)$ over the energy range of each group. Thus $\phi_g(\vec{r})$ denotes the flux $\phi(\vec{r},E)$ integrated over the range of energies E_g in the group $E_g \leq E \leq E_{g-1}$. Then, we have to derive equations governing the behaviour of $\phi_g(\vec{r})$. We will find that these equations take the form of a set of diffusion equations describing the neutrons in each energy group.

The equations are coupled to one another since neutrons may undergo changes in energy by, for example, being scattered from one group to another. Also, fission neutrons will usually appear in the highest energy groups and then cascade downward in energy as they are moderated by scattering collisions.

Recalling the rather detailed dependence of neutron cross sections on neutron energy E, one might expect that a great many such energy groups would be necessary to adequately describe the energy dependence of neutron flux. Surprisingly enough, however, most nuclear reactor calculations achieve sufficient accuracy using only few group diffusion descriptions. The validity of such a procedure depends critically on a judicious choice of the energy-averaged cross sections which characterize the neutrons in each group. Hence the determination of these group averaged cross sections or parameters is the key to the successful implementation of multigroup diffusion theory.

We will first give a heuristic derivation of the multigroup diffusion equations based on the concept of the neutron balance. Before these equations in a more rigorous manner which further will enable us to ascertain the validity of the multigroup diffusion approximation and will provide us with a basis for the calculation of coupled group diffusion constants.

Let us now consider a volume element ΔV about the point r in which we wish to derive the multigroup diffusion equation for the neutron balance for a given energy group g. Figure 1 shows the various ways in which neutrons can enter or leave the energy group g during the time interval Δt.



Before we begin our derivation, it should be appreciated that such a procedure would need at least the following

[illegible] = [absorption in group g] + [source neutrons appearing in group g] − [neutrons scattering out of group g] + [neutrons scattering into group g] − [illegible]

From now on we will speak of group i instead of group g.

It should be noted that we have taken explicit account of the fact that a scattering collision can change the neutron energy and hence can either remove it from group i, or if it is initially in another group j, scatter it into energy group i. We will denote by $\Sigma_R^{j\to i}$ the probability for scattering a neutron from group j to the group i, an $\Sigma_R^{i\to i}$. Then:

$$\Sigma_R^{i} = \sum_{\substack{j=1 \\ j\neq i}}^{M} \Sigma_R^{i\to j} \qquad (3\text{-}3)$$

becomes the cross section for removal from group i.

We will similarly define an absorption cross section which includes the group i, Σ_a^i, and a source term $S^i(x)$ giving the number of neutrons appearing within this group. We will also associate with each group a diffusion coefficient D^i so that the leakage from the group can be written within the diffusion approximation as $-D^i\nabla^2\phi^i(x)$. By combining all of these terms, we find a multigroup diffusion equation of the time independent balance equation form which can be solved by Eq. (3) and thus:

$$\left[-\nabla\cdot D^i(x)\nabla + \Sigma_a^i(x) + \Sigma_R^{i\to i}(x) + \sum_{\substack{j=1\\ j\neq i}}^{M}\Sigma_R^{i\to j}(x)\right]\phi^i(x) =$$

$$\sum_{\substack{j=1\\ j\neq i}}^{M} M^{j\to i}(x) + S^i(x) \qquad (3\text{-}4)$$

$$M^{j\to i}(x) = \frac{\chi^i}{\sum_{k=1}^{M}\chi^k}\sum_{k=1}^{M}\nu\Sigma_f^k(x)\phi^k(x) \qquad \text{(fission source term)} \qquad (3\text{-}5)$$

$$S^i(x) = \sum_{\substack{j=1\\ j\neq i}}^{M}\Sigma_R^{j\to i}(x)\phi^j(x) \qquad \text{(removal source term)} \qquad (3\text{-}6)$$

Here we have the spatial variables, either x-y or r-z, and M is the total number of groups. The most general combination of these symbols are

D^i: the diffusion coefficients

ϕ^i: the neutron flux

Σ_a^i: the macroscopic absorption cross section

Σ_r^i: the macroscopic removal cross section from group i

$\Sigma_r^{i\to i'}$: the macroscopic removal cross section from group i to group i'

B_t^2: the geometric buckling in the transverse direction

χ^i: the probability that a fission neutron will be born with energy in group i

$\nu\Sigma_f^i$: the macroscopic fission cross section times the average number of neutrons per fission

λ: the eigenvalue

Hence we now have a set of NG coupled diffusion equations for the NG unknown group fluxes $\phi^i(x)$.

The major sections of MIMBUS perform the following functions:

1. Processing of the input data, including checking and editing.

2. Calculation of the required macroscopic cross sections for group structure G.

3. Calculation of the coefficients for the finite difference equations used to approximate the group diffusion equations, including boundary and boundary conditions.

4. Solution of the eigenvalue problem represented by these finite difference equations.

5. Calculation of the fuel depletion and accumulation of fission products for a specified time step.

6. Printing of selective information for printing and plotting.

In order to have MIMBUS readily modifiable for [illegible] to suit [illegible] of the IBM-360 system, both with [illegible] storage. The dimensions of the [illegible] of groups, compositions, regions, mesh points, [illegible] and so on, are parameters.

[illegible] values of these parameters, for the present version of MIMBUS, are given in appendix B.

A brief description of the physical model employed is given [illegible] the history of core life, the elements constituting [illegible] are uniformly distributed, but as a result of [illegible] depletion become non-uniform. Hence, in [illegible]

to take into account the spatial variation of the group constants, namely, the diffusion coefficient D_g, the fission cross section $\nu\Sigma_{fg}$ and the neutron production rate per unit of flux $\chi\Sigma_{fg}$.

The spatial dependence of these group constants is realized by dividing the reactor into an arbitrary number of regions of arbitrary shape. Each region is considered as a homogeneous mixture of fuel, that is all the isotopic number densities are considered as uniformly distributed within the same region.

CHAPTER II

EREBUS consists of one main program and thirty-three sub-programs. The [illegible] diagram of EREBUS is given in Figure II-1. The main program calls the subprogram OVER-1, OVER-2, ... OVER-7. It controls the number of time steps. If time step number (ISTEP) is greater than the last time step number (ESTEP) then the program is terminated.

Program is terminated when the convergence is attained. For the termination of the problem subroutine EXIT is called.

II-A SUBROUTINE OVER-1

In order to have EREBUS readily modifiable for adaptation to other machines of the IBM-360 series, but with different maximum storage availabilities, the dimensions of the [illegible] are variable. Before the title card two input cards have to be read which contain the values of the parameters specifying the dimensions of the problem. The meaning of the quantities are

MXLS:	Maximum	number	of	library sets
MXSS:	"	"	"	self shielding sets
MXCO:	"	"	"	compositions
MXGS:	"	"	"	groups
MXFI:	"	"	"	fuel isotopes
MXFR:	"	"	"	fission products
MXIS:	"	"	"	isotopes
MXBI:	"	"	"	burnable isotopes
MXTS:	"	"	"	time steps
MXCR:	"	"	"	control rods
MXCB:	"	"	"	control banks
MXRG:	"	"	"	regions
MXTS:	"	"	"	small time steps
MXTB:	"	"	"	elements in the control list
MXIX:	"	"	"	X meshes
MXIY:	"	"	"	Y meshes
MXSC:	"	"	"	self shielding coefficients

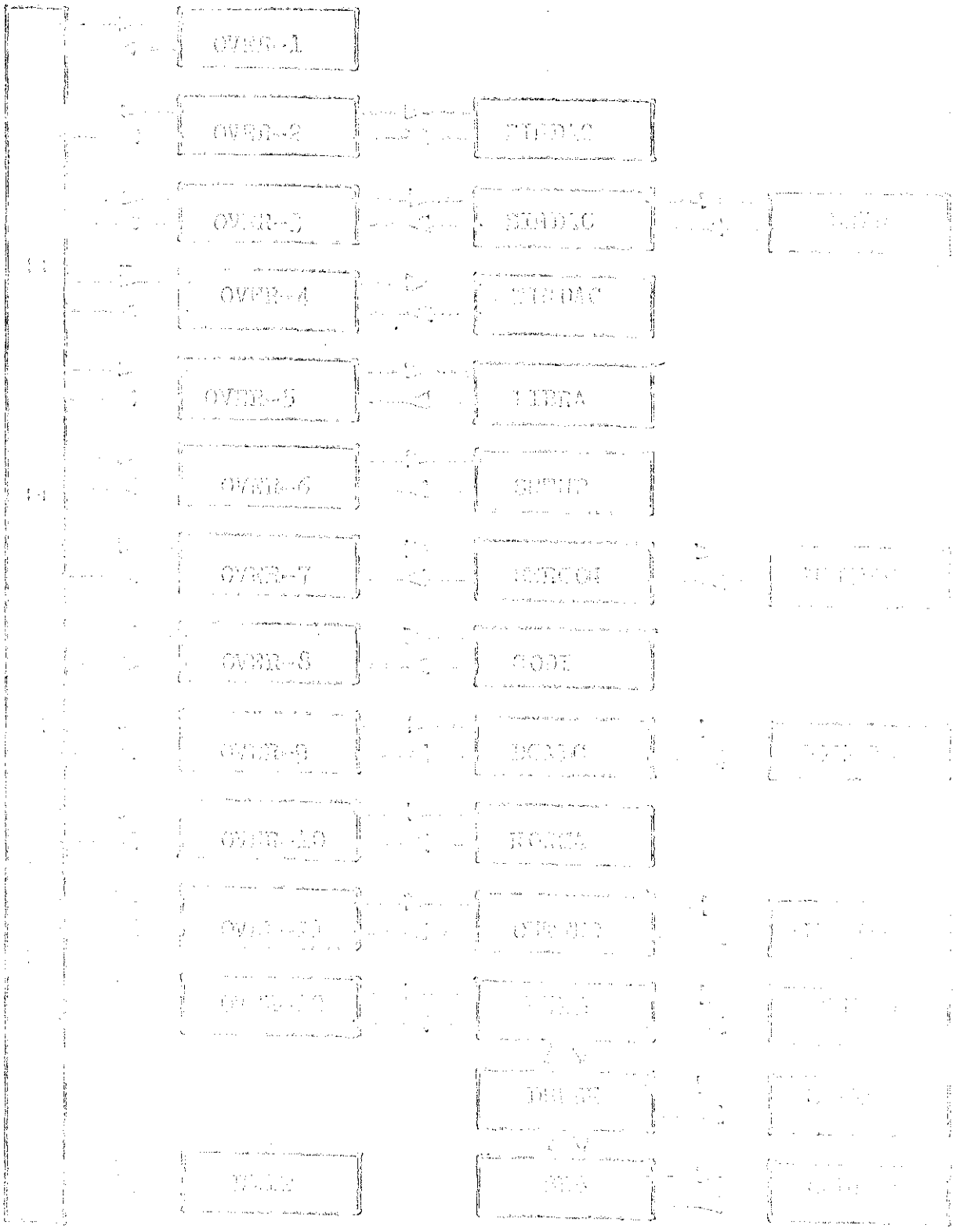


Figure 1.1 The schematic diagram of MMWVS

KPD: Maximum number of mesh points
IPR: " " " print indices
IOF: " " " arrays taken in common

The following conditions have to be observed:

KIF≥KIF	KIF≤KCD
KIV≤60	KLEFT≥5
KXD ≤KYD	KROD≥5
KCD≤KREG	KBRL≥5

NPP≥NPX·NPY or (KXD·KYD)

LBD ≥(NPX + 1)·NPY/2 or (KXD + 1)·KXD/2 for diagonally symmetric problems.

$$KOF \geq NG \cdot NCP \sum_{i=1}^{NPP} NPT(I)$$

where

NCP: Number of the coefficients
NPT(I): Number of blocks of self shielding coefficients of the set I

The values of the above parameters are printed on output by OVERLAY. The length of the common region is calculated and is printed out. Subsequently a return is made to the main. Variable IERR is zero. If variable errors and if IERR>0, then appropriate error

CHAPTER III

The first stage in a reactor code is to read in the data. This data can usually be presented in some compact form. Hence, the data is scrutinized for any possible errors and utilization of any leads to an abortion.

MERGE is an "overlay program" constituted by main and subprograms which are illustrated in Figure III-1. Subprograms OVER-2, OVER-3, ... , OVER-12 are used only to call various subprograms. Subprograms FINDAC, FINDAC, READR, FINDAC are used to read, check, reorder and print out the input data. The input data have been divided into 35 card sets. Each set may contain one or more cards. Input data set is given in APPENDIX-I.

There are three types of starts in MERGE for each one of which a different input set is provided.

a. Normal start: We will deal with normal start in our study.

b. Strong restart: With this type of restart, a problem interrupted during the finite difference calculation by a malfunction, can be restarted from the last point (or the last but one,) written by liberation being performed at the time of interruption.

However, if the restart is made using also the flux tape, prepared by the program, the MERGE RESTART is considerably shortened. The restart of a problem from the every point is done at the beginning, except for a loss of the negligible work. Such is the actual computational time.

c. Weak restart: By this type of restart, a problem can be restarted at the nodal edges (surfaces), which is the case when a control blade steps, or by any other possible, physical.

III-A FINDAC

FINDAC is the subprogram referenced by OVER-2.

The geometric specification of the reactor is given as

input data in this subprogram. The x axis (or the r axis in cylindrical geometry) is coincident with the top side of the reactor and is rightwards oriented. The y axis (or the z axis in cylindrical geometry) is coincident with the left side and is downwards oriented. From now on we will speak of x,y axis, also for the cylindrical geometry.

In the mesh grid layed out for the finite difference discretization, the lines parallel to the x axis are called rows and the lines parallel to the y axis are called columns.

Rows and columns are numbered, starting from 1, from top to bottom and from left to right respectively. This is shown in Figure III-1.

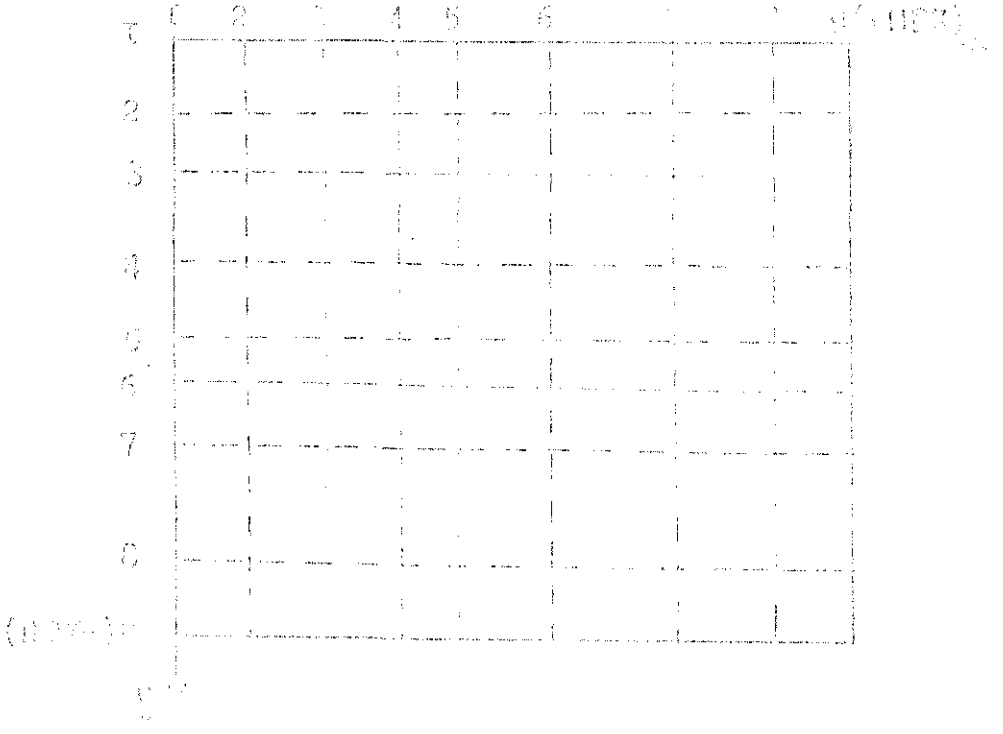


Figure III-1 Sample reactor core mesh layout

The reactor is divided into regions in each of which the neutron spectrum is assumed homogeneous, that is, constant and hence the same macroscopic cross sections in all rectangular meshes belonging to a given region. A region can also be made up of disjoint sets of mesh cells (meshes).

Two or more regions can have the same initial composition. In the following and also in the program print-out, the initial composition will be simply named composition. But, after the first burn-up interval is elapsed, and the isotopic number densities have changed, each region generally represents a new composition.

III-A-1 BOUNDARY CONDITIONS

The boundary conditions are given as

$$\alpha^i \phi^i + \beta^i D^i \frac{\partial \phi^i}{\partial n} = 0 \qquad (i = 1, 2, \ldots, NG) \quad (III-1)$$

through which the following cases can be specified.

1. Flux is equal to zero when $\alpha^i \neq 0$ and $\beta^i = 0$ (zero flux condition).
2. Current is equal to zero when $\alpha^i = 0$ and $\beta^i \neq 0$ (zero current condition).
3. Current condition $\left(-D^i \frac{\partial \phi^i}{\partial n}\right) \neq 0$ when $\alpha^i \neq 0$ and $\beta^i \neq 0$.

If $\left(\frac{\alpha^i}{\beta^i} = 0.5\right)$ and $\beta^i = 1$ condition (III-1) represents a variable in the sub zero extrapolated current in diffusion theory.

This last condition should be employed when the actual core dimensions rather than the extrapolated ones are being used for one of the batch cases of variable flux. For the boundary condition specification, the boundaries are numbered counterclockwise starting from the top side as shown in Figure III-2.

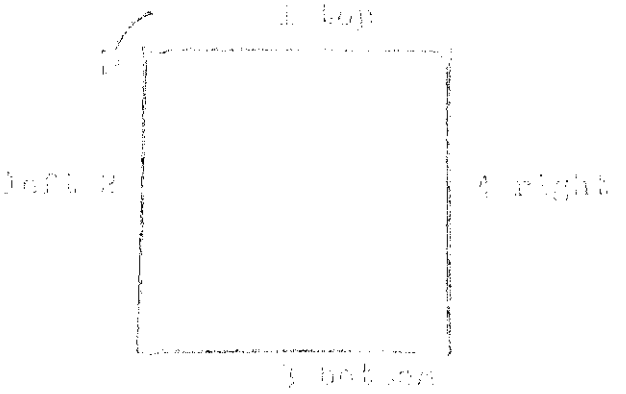


Figure III-2

Boundary conditions may be group dependent or independent. If the boundary conditions are group dependent, then as many as IG (number of groups) cards must be supplied, one for each group. If it is group independent, usually the case for all groups, then only one card is necessary and specified values apply to all groups.

If $\alpha\hat{\Omega}\cdot\hat{p}^{\perp}<0$, the program will stop, except when this condition occurs on the left side of a cylindrical or spherical geometry. In this case the program sets automatically $\alpha\hat{\Omega}\cdot\hat{p}=0$ and $\gamma=1$ (symmetry condition)

If zero current condition occurs at any boundary, then the program sets the boundary condition indicator as zero for this group and this side.

If zero flux condition occurs at any boundary, then the boundary condition indicator is set to be minus one for this group and this side.

For the vanishing condition (vanishing inward current), it sets the indicator as $\alpha\hat{\Omega}/\beta$. This location must always be greater than unity.

III-6 SUBROUTINE SINBAC AND OUTP

These subprograms read, check, recorder and print out region-wise the basic input data for the geometric specification of the problem. Input data to the subprogram SINBAC, the first subroutine used, are called mesh specifications, and are described in sec.

The geometric specification of the regions in each direction (the input is mandatory" called mesh specifications and are described in sec. 2) for the computation space (the region is inputted by a group of input data, each of which gives the limits of a line region (mesh), for all mesh lines successively or particularly the preceding ones.

This may be figure III-3, the regions are numbered in the direction is considered as follows:

Suppose the regions were divided into 9 regions. In each of them the mesh is to be given as merge boundary, that is, only the mesh lines or boundaries which are changing in the successive order, beginning to all subsequent ones have to be given region. Vertical (columns) and horizontal (rows)

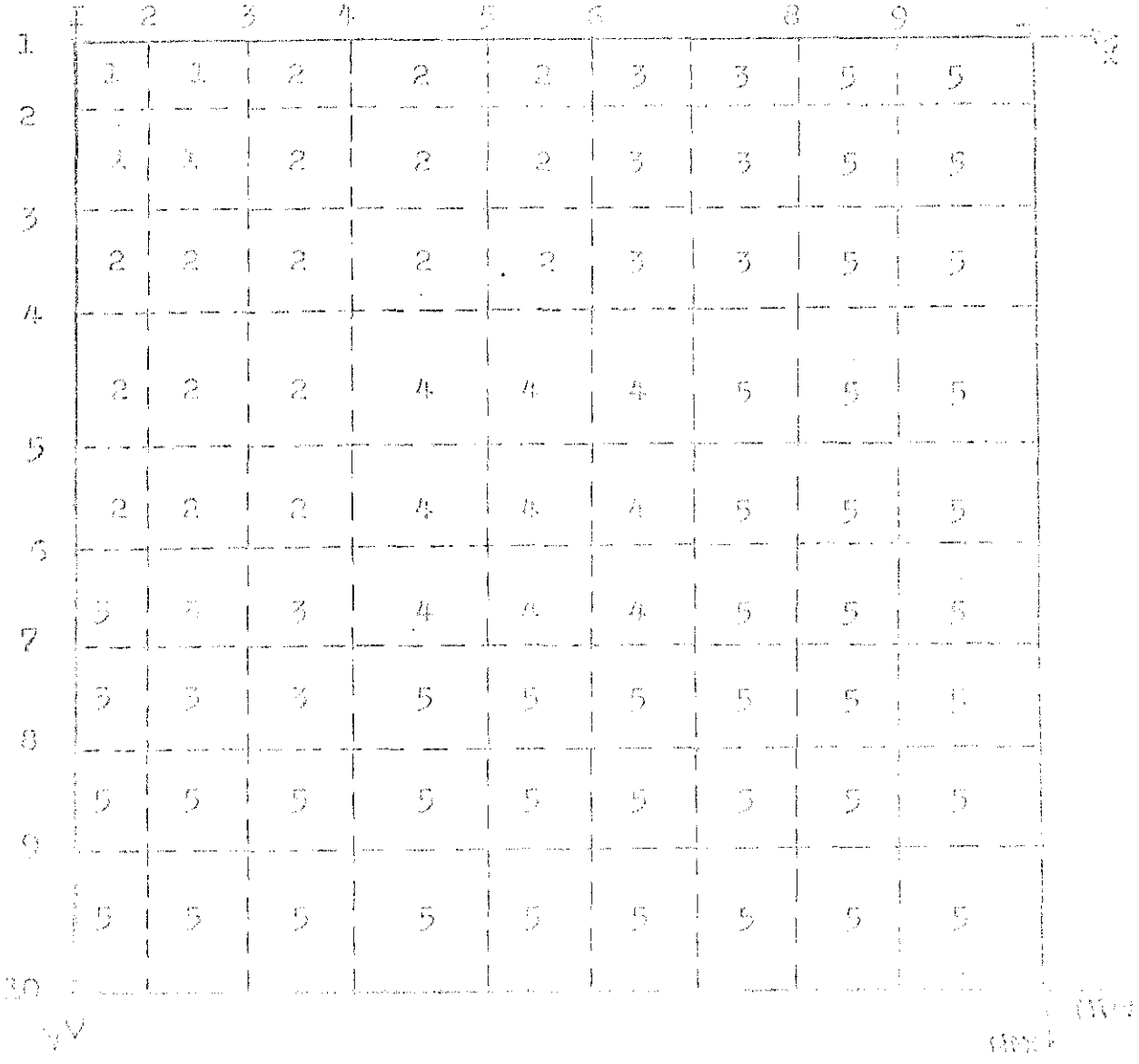


Figure III-3 Example reactor core region system.

lines are drawn at all the region interfaces. The remaining blocks are used as regions. In this section the number of each interface and the width of each vertical region going from left to right are specified, followed by the number of interfaces and the width of each horizontal region going from top to bottom. The inputs for the regions shown in Figure III-3 would be as follows

R E G I O N O V E R L A Y

Region number	Column number	Row number
5	1 – 10	1 – 10
4	3 – 7	4 – 7
3	1 – 4	1 – 4
2	1 – 6	3 – 6
1	1 – 3	1 – 3

Subprogram SIZDAC calculates the region and composition mesh sizes. Each region length between zero to Δy and each mesh Δx, Δy other dimension is unity. Then the volume of one such mesh is

$$VOL = \Delta x . \Delta y \qquad (D-2)$$

A region or mixture of one or more such squares, the volume of the region is found by summing over the mesh area volumes which belong to the same region. The same way is used to calculate the composition volumes. VOL(k) is the volume of region k.

After the region volumes, composition volumes are calculated by the same way by summing up to the region volumes for the composition as we do to obtain the composition volumes. VOL(k) is the volume of composition k.

EXTENDED NUCLIDE CHAIN SPECIFICATION

Fuel depletion analysis is concerned with predicting the isotopic concentrations in reactor fuel compositions as a function of irradiation. During nuclear operation, such changes have significant bearing on the operating life of a reactor, as well as on its reliability and control.

A wide variety of nuclear processes must be considered during fuel depletion analysis. These include, of course, the usual fission and absorption reactions. However, one must also account for the transformation of fissile nuclides into fissile isotopes and for the creation of numerous fission products. Finally, one must account for the reversibility between the various nuclides. For example, the capture of a neutron by U^{238} produces U^{239}, which decays to Np^{239} and then subsequently decays to Pu^{239}. Thus, U^{238} is a source for Pu^{239}.

A complete burn-up calculation would involve the solution of the coupled reaction rate equations describing such processes for the hundreds of different isotopes in a reactor core. In practice, one usually introduces approximations that greatly simplify these calculations. For example, the only fission products that are explicitly treated are usually those with large capture cross sections and fission yields, namely, Pr^{149}, Sm^{149}, I^{135}, and Xe^{135}. The remaining fission products are lumped into one or several groups, each characterized by an effective cross section. Furthermore, any nuclide with a short half life is omitted from the burn-up calculation.

The specific isotopes considered depend on the particular fuel used in the core, the isotopes of interest in both U^{233}-Th and Uranium-Plutonium fueled reactors are indicated in Tabl 1 and 2 respectively.

TABLE 1

No	Name	Will couple to proc	Not capture in proc	Very volatile	Chemically separable	Is very important
1	U-233	-	-	-	Yes	No
2	U-236	-	-	-	Yes	No
3	U-238	-	-	-	Yes	No
4	Np-239	-	-	-	Yes	No
5	Np-240	-	-	-	Yes	No
6	Pu-241	-	-	-	Yes	No
7	Pu-240	-	-	-	No	Yes
8	Pu-242	-	-	?	Rel	Yes
9	Am-243	-	-	-	No	Yes
10	Cm-245	-	-	0	No	Yes
11	Some of the other products	-	-	-	No	Yes
12	Rare	-	-	-	No	No
13	Remainder of fission products	-	-	-	No	Yes

TABLE-2

No	Name	1st capture parent	2nd capture parent	Decay parent	Absorbable	Fissionable
1	Th-232	--	--	--	Yes	No
2	Pa-233	1	--	--	Yes	No
3	U-233	--	--	2	Yes	No
4	U-243	3	2	--	Yes	No
5	U-235	--	--	--	Yes	No
6	U-236	5	--	--	Yes	No
7	U-238	--	--	--	Yes	No
8	Np-239	7	--	--	Yes	No
9	Pu-239	--	--	8	Yes	No
10	Pu-240	9	8	--	Yes	No
11	Pu-241	10	--	--	Yes	No
12	Pu-242	11	--	--	Yes	No
13	Pm-149	--	--	--	No	Yes
14	Sm-149	--	--	13	No	Yes
15	I-135	--	--	--	No	Yes
16	Xe-135	--	--	15	No	Yes
17	1st group of fission product	--	--	--	No	Yes
18	2nd group of fission product	--	--	--	No	Yes
19	3rd group of fission product	--	--	--	No	Yes
20	Boron-10	--	--	--	No	No
21	Burnable poison	--	--	--	No	No

The initial flux approximations and bucklings are given as inputs Subprogram SINDAC defines the initial fluxes and bucklings for each region and writes them on the logical unit 5.

The number densities of the fissile isotopes (that is, the time dependent isotopes, plus control isotope) can be specified either per composition or per region or both. The number densities of the time independent isotopes except for Sh-[illegible] (the control isotope) can be specified only per composition.

In the criticality searches by means of a control isotope variation (ICRISW = 1,2 on card no.3 columns 28-30), the fissile isotope assumes, as control isotope, the isotope no [illegible].

We recall that the number densities, both per composition and per region and the logarithmic derivatives, are all set equal to zero before any reading, except in the restart problems. In the latter case, the number densities and the logarithmic derivatives are the ones read from the restart tape.

III-C SUBROUTINE SINDAC

The goal of this subprogram is to read, control, reorder and print out the input data the list of which is given in Appendix A.

ERGOS can solve at each time step, four types of diffusion calculations. The required input data is provided in this subprogram. If there is any error in input then program gives a clarifying error message.

Types of diffusion calculations are classified as follows:

a. Straight diffusion calculation.
b. Criticality search by uniform variation of a control isotope.
c. Criticality search by a programmed regionwise variation of a control isotope.
d. Boundary search.

These will be explained in chapter V.

SINDAC also computes the average fluxes for each mesh point. If input flux approximation is negative at some points or zero at every point then this problem can not be continued. On the other hand, input flux approximation for all mesh points are written on logical unit [illegible], and printed out.

troduce λ, the multiplication fact
the fission chain reaction and th
ation rate of fissile atoms, so
ow in such a way that the number of
s are balanced by the rate of fi
ns express this requirement in
the neutrons play the central role
he reaction let us focus our att
a given neutron will be "born" i
ously sentence about the life
h role" in either an absorp
by neutron. Certain
, fissile or fissionable nuclei and
ously leading to the birth of new
new "generation" of neutrons. Sup
s is the number of neutrons
will then define the rate of
ation factor λ characterizing the

$$\text{Multiplication factor} = \frac{\text{[illegible]}}{\text{[illegible]}}$$

ares the number of fission neutron
ceed to the number of fissions
ion (recall that each fission
nuclei neutrons), we could
the number of fission
ve left unsaid, however,
ed in the reaction. Only
ssion fission
reaction, either
ing fissions, for
ions of U^{235}, but with
ther or lack out of the

p neutron inhibits or
ges the birth of neutron

ion is reached in the
ission that is

ut if $\lambda=1$, the number of
ion sites will be the
ill be kept under control. We

[illegible] by $\lambda=1$ as being critical. Hence the [illegible] of the nuclear engineer is to design the [illegible]. One possible approach would be to [illegible] nuclear material composition and configuration [illegible] for this choice, and if λ is not unity, [illegible] won't be on the first try, readjust the [illegible] design until the criticality condition, [illegible]

[illegible] adjustment of the core composition is through the [illegible] control poison density without which the [illegible] k thus allowing for a margin of excess [illegible] and more importantly for reasonably long [illegible]

THE SUBROUTINE LIBRA

[illegible] essentially two types of nuclear reactions [illegible] in the study of nuclear reactors:

1. [illegible] reactions resulting from the collision between [illegible] nucleus,

2. [illegible] spontaneous disintegrations of nuclei.

[illegible] neutron-nucleus collision events involved [illegible] Let us consider an example of the first type of [illegible] reactions depend not only on the [illegible] conditions, as in the case of the [illegible] on the relative velocity with which [illegible] An example of the second type of [illegible] is the decay of fission products, since [illegible] rate.

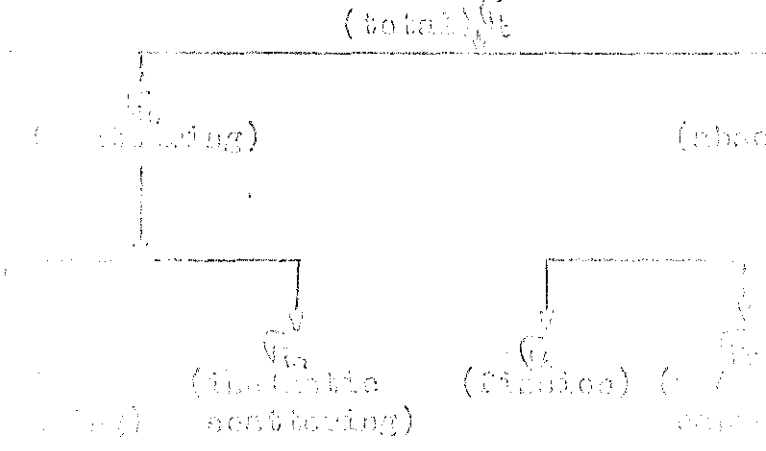
[illegible] the wide variety of possible nuclear [illegible] which is inherent in the [illegible] neutron into nations between [illegible] a neutron-nucleus [illegible] of nuclear cross sections. [illegible] 10^{-24} cm^2 and the geometrical [illegible] of the order of 10^{-24} cm^2. [illegible] cross sections would be [illegible] cm^2. However this generality [illegible] reaction can reasonably be [illegible] larger or smaller than the [illegible] values due to resonance effects [illegible] energy mechanical nature of the [illegible] nucleus. For example, the absorption [illegible]

for slow neutrons is almost one million to
...sectional cross section.

...by such cross sections can be used to ...
...nuclear reaction, thus the definition ...
...reactions for each type of neutron-...
...different nuclei. For example, ...
...sorption and scattering are denoted by ...
...respectively, we can introduce the ...
...related to the probability that ...
...reaction will occur, or, formally

$$\sigma_t = \sigma_a + \sigma_s = \sigma_e + \sigma_{in} + \sigma_\gamma + \sigma_p + \sigma_{an} + \ldots$$

...diagram of the hierarchy of ... conventional notation is shown in Fig. ...



...ETI-4 Neutron cross section hier...

...have defined the concept of ...
...ing the neutron ...
...the basic ...
...such ...
...type of ...
...sections. For ...
...ng, a very strong ...
...the neutron cross ...
...ility with carbon and ...
...ear applications.

[illegible] LIBRARY SET

[illegible] scopic cross section tape for this [illegible] codes but, GRIS, developed by [illegible] under the auspices of [illegible] Verbung in Schiffbau und Schiffahrt [illegible] ifically for this purpose.

[illegible] ation of the actual microscopic cross [illegible] to divide the energy spectrum [illegible] is divided into 45 micro groups and the [illegible] for all the micro groups are supplied [illegible] groups can be condensed up to [illegible] group data is generated by GRIS [illegible] to 35 in the present version of [illegible] stored in the RUFUS file [illegible] FERM. Thus, it is possible [illegible] of microscopic cross section [illegible] set is outlined in Figure [illegible] to assign each initial composition to a [illegible]

[illegible] number (REL) is greater than [illegible] supplied consecutively by [illegible] order in which such [illegible]

[illegible] SHIELDING SET

[illegible] reactor core is not homogeneous [illegible] the self shielding [illegible]

[illegible] of self shielding factors [illegible] called the [illegible] provided as input, as will be [illegible]

[illegible], in RUFUS, to specify [illegible] self shielding [illegible] each initial composition to a [illegible]

Isotope Index	Nuclear Data
1	σ_{el}^{i} $i=1,2,\ldots,NS$ σ_{a}^{i} $i=1,2,\ldots,NS$ σ_{r}^{i} $i=1,2,\ldots,NS-1$ σ_{f}^{i} $i=1,2,\ldots,NS$ $\nu\sigma_{f}^{i}$ $i=1,2,\ldots,NS$ e^{i} $i=1,2,\ldots,NS$ $g^{(k-1)}$ $k=1,2,\ldots,NG+1$ $\sigma_{s}^{i(k-1)}$ $k=1,2,\ldots,NG$ $i=1,2,\ldots,NS$
2	σ_{el}^{i} σ_{a}^{i} σ_{f}^{i} .
	σ_{el}^{i} σ_{a}^{i} .
NIS	σ_{el}^{i} .

Table 1 Tabulable representation of our Nuclear

[illegible] The specification of one self shielding [illegible] to one generic self shielding [illegible] shielding set (NSS≥1) are provided [illegible] which consecutively. Each set will be [illegible] (called the set number) according to [illegible] sets appear in the input deck.

[illegible] consists of NG,NGP coefficients. The [illegible] self shielding coefficients for a [illegible] group. Each self shielding set [illegible] the set of isotopes present in the [illegible] will be assigned. Number of sets [illegible] to each group is less than or equal to [illegible] to assign to each isotope a self [illegible] illustrated in Figure III-6.

[illegible] must have NG cards, one for each [illegible] the self shielding coefficients in addition to the total number of sets [illegible] such that

$$\text{NGP} = \text{NG}\cdot\text{NSP}, \quad \sum_{K=1}^{\text{NSS}} \text{NST}(K) \leq \text{KCOT}$$

[illegible] card version of MIXSG

[illegible] = 4000

[illegible] The subroutine MIXSA is to read [illegible] input data. If it [illegible] of subtask is discontinued.

[illegible] sets and self shielding [illegible] to the self shielding [illegible] will be generated [illegible] the calculation of [illegible] concentrations for [illegible] will also be [illegible] of course, to do this [illegible]

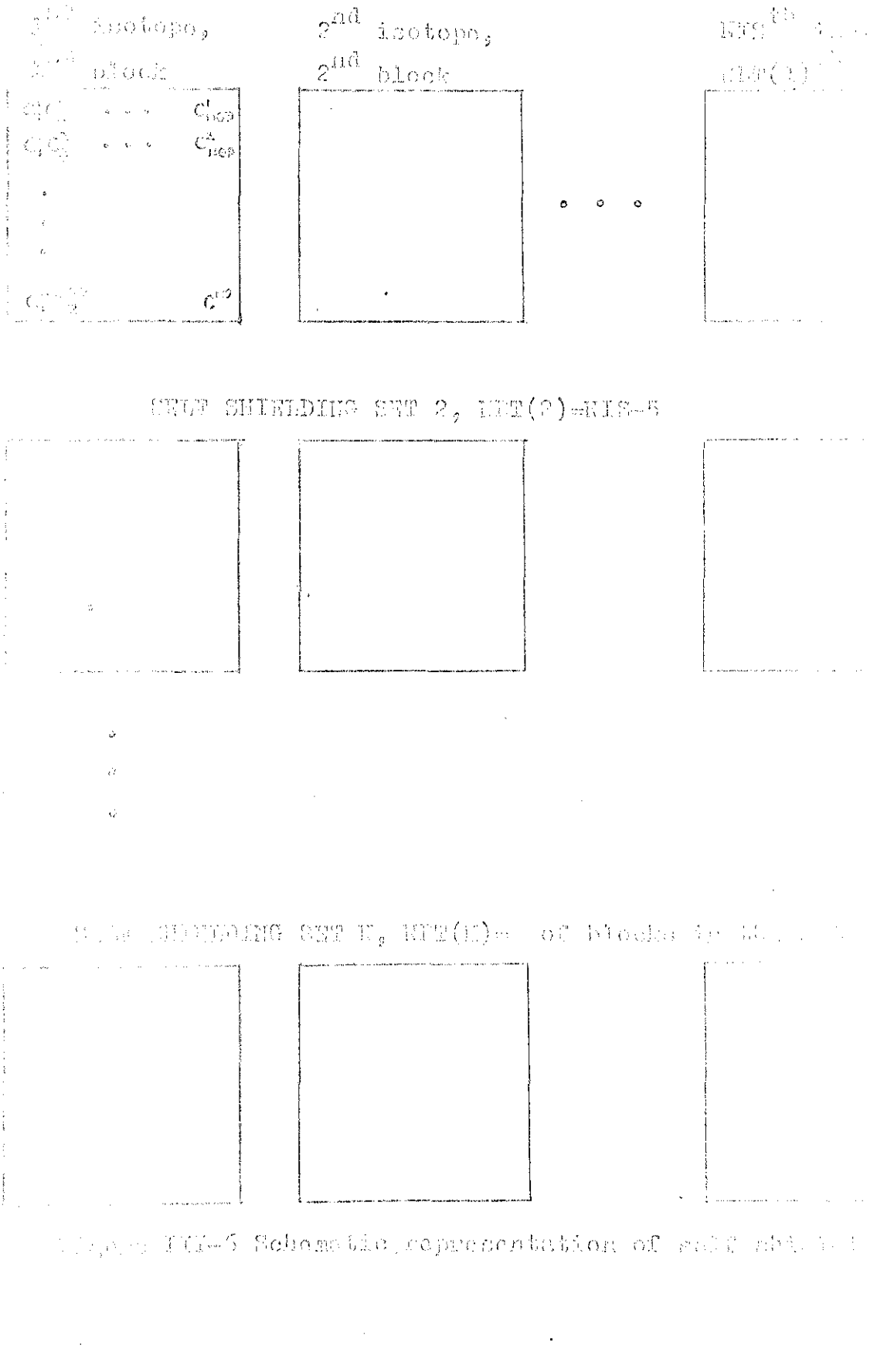


Figure 7(1-5 Schematic representation of self shi

CHAPTER-IV

The product of the atomic number density N and the [illegible] cross section σ_k is denoted by Σ_k. It is called [illegible] cross section

$$\Sigma_k = N\sigma_k = \frac{\text{[illegible]}}{cm^3} \cdot cm^2 = cm^{-1} \qquad (4.1)$$

[illegible] to Σ_k as the total macroscopic cross section [illegible] target material, whereas the microscopic [illegible] to the probability of [illegible]. It should be noted that Σ_k [illegible] cm^2, since its unit is [illegible]

[illegible] has been restricted to total [illegible] characterize the probability [illegible] of reaction. We can go [illegible] ing the macroscopic cross section [illegible] on the microscopic cross section [illegible] multiplied by the number [illegible] of nucleus. For example, the [illegible] would be defined as

$$\Sigma_{in} = N\sigma_{in}$$

[illegible] of a macroscopic cross section [illegible] cross sections of different [illegible] inelastic cross section σ_{in} [illegible] of elastic cross section σ_{el} [illegible] cross section σ_t is [illegible]

$$\Sigma_t = N_1\sigma_1^t + N_2\sigma_2^t + N_3\sigma_3^t \qquad (4.2)$$

[illegible] the microscopic cross section for nuclide [illegible] non-nuclear reaction cross sections depend [illegible] energy of the incident neutron.

[illegible] the macroscopic cross section can depend on [illegible] as well. For example, suppose that [illegible] uniform composition, then the macroscopic [illegible] will be space dependent. In a similar [illegible] position might depend on time. Suppose, for [illegible] the nuclide of interest is unstable such that it [illegible] decaying as a function of time. Therefore, in [illegible] case, one would write

$$\Sigma(r, E, t) = N(r,t)\sigma(E) \qquad (7.$$

to indicate the explicit dependence of the macroscopic [illegible] on neutron energy E, position r, and time t.

In the next two sections, first the number density [illegible] burnup, after that, macroscopic cross sections [illegible]

[illegible] NUCLEOSYNTHESIS SETUP

[illegible] number densities of burnable isotopes [illegible] decay constants, are read from the [illegible] variable NUD = 0. Those number densities [illegible] unit number 10 initially as input at the [illegible] month for the following time steps.

[illegible] variable NUD is increased by 1 so as to be [illegible] variable isotopes. Calculation of the [illegible] is for each region as follows

$$\gamma(I,J) = \frac{N(I,J)\cdot V(I)\cdot A(J)}{AV} \qquad (7.$$

[illegible]

[illegible] = Burnable (time dependent) isotope

[illegible] = number density of the J^{th} isotope in [illegible]

[illegible] = volume of the I^{th} region (cm^3)

[illegible] = atomic weight of the J^{th} isotope (gm/mole)

[illegible] = Avogadro number ($\#/cm^3$)

[illegible] = weight of the J^{th} burnable isotope in [illegible]

[illegible] = 2 the same calculation is made to obtain [illegible]

of burnable isotopes in composition M.

$$W(M,J) = \sum_{L} \frac{N(L,J) \cdot V(L) \cdot A(J)}{Av.}$$

the composition M consists of regions denoted by

calculates the total weight of each burnable

$$W(J) = \sum_{L=1}^{NREG} \frac{N(L,J) \cdot V(L) \cdot A(J)}{Av.}$$

on a tape file the data required

microscopic nuclear data, bucklings,

coefficients, and number densities.

, if there is fuel shuffling, then

burnable isotopes in the

region or composition.

only if the time step number is

shuffling has been effected then a

in which case the subprogram

of the isotopes in each region and

THE SUBROUTINE SERCON AND SAPPTO

determining the type of the criticality

of start, this subprogram

of the reactor core, one

and the other doing the same

the criticality search,

calculates the

tions and prints out the

solves, at each time step, four types

cases are classified as follows:

THE SUBROUTINE DIFFUSION CALCULATION

solves the solution of the diffusion

[illegible] the eigenvalue λ_0 which is coincident with the [illegible] of the reactor. This type of [illegible] called "Straight Burnup".

[illegible] CRITICALITY SEARCH BY UNIFORM VARIATION [illegible] ISOTOPE

[illegible] is the search of a prefixed multiplication [illegible] uniform variation of a control [illegible] the number density of the control [illegible] in each region, except for a suitable [illegible] the dilution factor, unique for the whole [illegible] is calculated by the program between [illegible] Θ_{min} and Θ_{max} are to be input. The [illegible] is given as input.

[illegible] first determine the eigenvalues [illegible] Θ_{max} and Θ_{min}. If $\lambda_1 > \lambda_c$ and $\lambda_2 < \lambda_c$ [illegible] first estimate $\Theta^{(1)}$ is determined by the [illegible]

$$\Theta^{(1)} = \Theta_{min} + (\Theta_{max} - \Theta_{min}) \frac{\lambda_1 - \lambda_c}{\lambda_1 - \lambda_2}$$

[illegible] process is carried out, by successive [illegible] two consecutive couples of λ [illegible] is found such that

$$|\lambda^{(r)} - \lambda_c| < \eta$$

[illegible] is not equal to $\Theta^{(r)}$ and the search in [illegible] sensitivity ξ_i does not change significantly [illegible] critical search is interrupted [illegible] final cells of a normal [illegible] a composition interpolation [illegible] this step.

[illegible] CRITICALITY SEARCH BY A PRESCRIBED VARIATION OF A CONTROL ISOTOPE

[illegible] sections is given in input. The [illegible] zone in each a link. One [illegible] link is to be changed, and such [illegible] A control rod is composed of a [illegible]

[illegible] control isotope is changed simultaneously by [illegible] according to the zone control laws, the [illegible] and minimum values, H_{max} and H_{min}, of [illegible] density, must be supplied for any of the [illegible]

[illegible] suppose now that, following the given [illegible] for operating a given control [illegible], [illegible] the eigenvalues λ and λ_c [illegible] of the reactivity $\delta\lambda = \lambda - \lambda_c$ does [illegible] to H_{max}, the critical value H_c [illegible] successive linear interpolation, [illegible] method for the determination of the [illegible] function f.

[illegible] the contrary, the reactivity $\delta\lambda$ [illegible] of the criticality cannot be achieved [illegible] zone operation, the program [illegible] control banks, as indicated by the [illegible]

[illegible] control bank is exhausted, the [illegible] of the problem ends with the [illegible] Regarding the number [illegible] the regions not belonging to [illegible] operation, the following rules [illegible]

[illegible] control banks, which include the [illegible] bank under examination, [illegible] the region taken the value H_{max} of [illegible] region appears;

[illegible] control banks, which include [illegible] bank under examination, [illegible] the value H_{min} of the first [illegible]

[illegible] of the control banks, [illegible] other case for the [illegible] to this region taken [illegible] control banks.

[illegible] to point out that, [illegible] region appears in [illegible] in one bank should be [illegible] in order to make sense from a [illegible]

[illegible] BOUNDARY SEARCH

[illegible] is the search of a predicted multiplication [illegible] of a quasi-continuous movement of the boundary of [illegible] zones of rectangular shapes.

[illegible] such control areas, the region of the [illegible] be specified. The follower explores the [illegible] moving boundary (its bottom side) in [illegible] the negative sense of the y axis).

[illegible] movement of the moving boundary from one [illegible] upon one, constitutes the elementary step of [illegible] search is performed in a specified quadrant [illegible] one (type III). A list of control points [illegible] are grouped into control banks, each [illegible] all control areas belonging to a bank [illegible] by therefore, an upper and lower limit [illegible] also be specified for each bank, within which [illegible] is confined.

[illegible] suppose now that, following the given [illegible] in searching a given control bank. The [illegible] moving boundary of each region of the [illegible] λ_{max}. Successively the boundary is displaced [illegible] this, and at each "elementary step" [illegible] test.

[illegible] is considered completed when a position [illegible] is reached, such that either the [illegible] the inequality $(\lambda_{max}-\lambda)<\varepsilon$ [illegible] conditions of the moving boundary.

[illegible] case, the critical boundary is not [illegible] which gives the smallest eigenvalue.

[illegible] moving boundary comes to the upper limit [illegible] of the two conditions which [illegible] with the same procedure for the [illegible]

[illegible], the position of the moving [illegible] to the one before the [illegible] is held.

[illegible] control banks, including the given [illegible] the moving boundary [illegible] the limit y_{max} of the last bank [illegible]

b. If the control banks, including the given area, [illegible] termination, the moving boundary of this [illegible] lower limit y_{max} of the first bank in which [illegible]

[illegible] case of the control banks, including th[illegible] the other ones follow the bank under [illegible] key of this area is set at the upper limit [illegible] the preceding banks.

[illegible] shows a reactor with 5 control areas. [illegible] constituted by areas 1, 2, 3, the second [illegible] the control limit is: 1, 2, 3, 3, 4, 5, [illegible] by the shadowed zones.

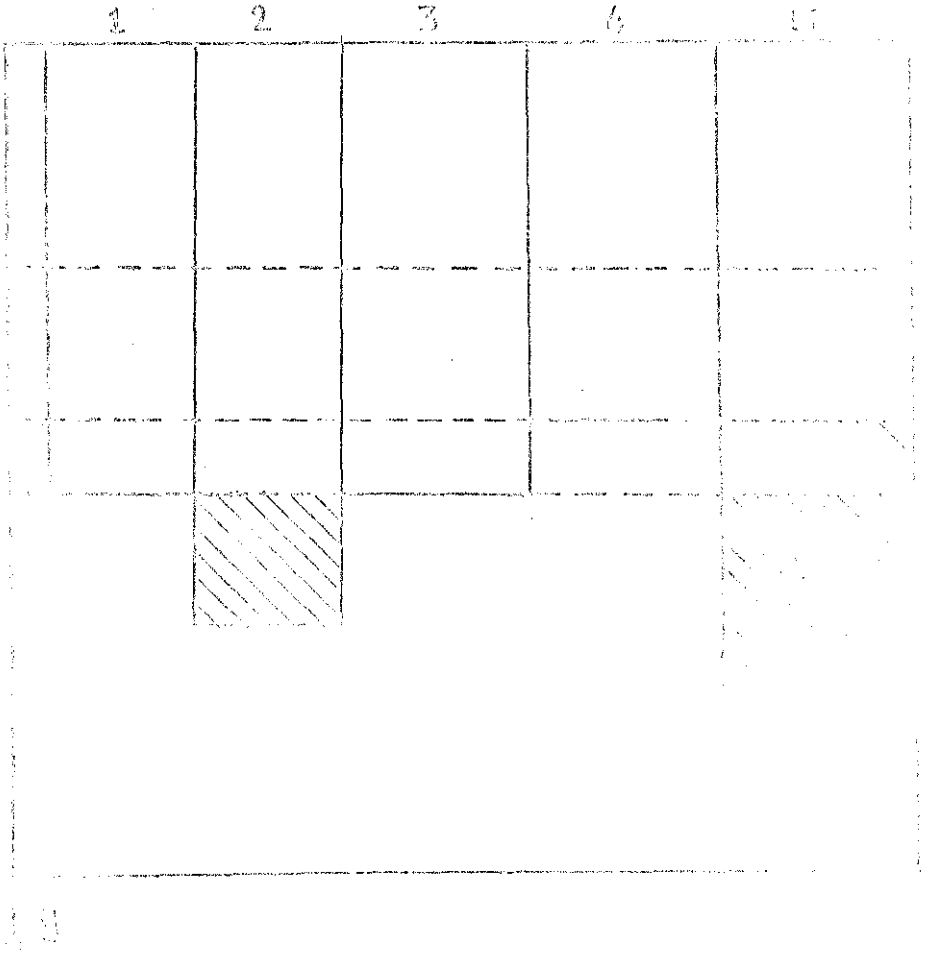


Figure IV-1 Example of control [illegible]

The criticality searches (ii), (iii) and (iv) are performed by means of a triple loop of iterations.

a. Criticality iterations: They are clearly described in sections IV-1-ii, iii and iv (in the boundary search (iv), an iteration is constituted by an "elementary step" of the searching boundary). The criticality iterations are interrupted when

1. The maximum number of outer iterations is exceeded,
2. The control list is exhausted,
3. The maximum number of criticality iterations is exceeded,
4. The reactivity $\xi\lambda$ in paragraph (ii) does not change sign when $\xi_{\lambda_{sup}}$ to $\xi_{\lambda_{inf}}$.

b. Outer iterations: They are defined in the same way as in most diffusion programs; the outer iteration is characterized by the successive estimates of the fission source and the eigenvalue λ, keeping fixed the boundary condition configuration.

Two criteria are employed to cease the outer iterations:

1. The eigenvalue convergence

$$\left| \frac{\lambda^{(k)}}{\lambda^{(k-1)}} - 1 \right| < 10^{-1}\eta \qquad (\ldots)$$

where η is the convergence criterion for the criticality and k the outer iteration index.

2. The pointwise convergence

$$\left| \frac{\varphi^{(k)}}{\varphi^{(k-1)}} - \lambda_{main} \right| < \varepsilon \qquad (\ldots)$$

where ε is an input "pointwise convergence criterion".

For any criticality iteration, the outer iterations are performed until condition (IV-10) is fulfilled, only if condition (IV-9) is achieved (or exceeded) at least once, the outer iterations may cease; condition (IV-9) is tested even if the criticality search is not over (2), (3), (4). If the search is over (1), the problem ends even if neither (IV-10) nor (IV-11). The outer iterations

coupled when the pointwise criterion (IV-11) is fulfilled.

... Inner iterations: The inner iterations are performed for the burnup of a given outer iteration in order to ... the group fluxes corresponding to the fission source of the outer iteration.

... calculation of type of straight burnup is performed ... inner and outer iterations only.

IV.F.4 CALCULATION OF THE SELF SHIELDING FACTORS

... the calculation of effective group constants it is necessary to generate self shielding factors as was described in the part IV.D.ii.

Self shielding factors $\xi^{i,j,l}$ are automatically calculated, on each time step by the semi-empirical relation

$$\xi^{i,j,l} = g^{i,j}\left(x^{i,j,l}\right) \qquad (IV-...$$

with

i = group index
j = isotope index
l = region index

... function $g^{i,j}(x)$ is given according to an option ... by ... of the following expressions. If the ... NN3(j) equals two or three, then the ...

$$g^{i,j}(x) = \sum_{n=1}^{n} c_n^{i,j}\, x^n \qquad (...$$

... NN3(j) equals zero or one, then the follow...

$$g^{i,j}(x) = \frac{c^{i,j}}{\sqrt{1 + \sum_{n=1}^{n} c_n^{i,j}\, x^n}} \qquad (IV-...$$

cross the independent variable is given according to another ... tion by either of the following expressions:

IF ITEM2(J) equals zero or two, then

$$\Sigma^{i,j,l} = \sum_{j=1}^{j} N^{j,l} \left(\sigma_a^{i,j} + \sigma_r^{i,j} \right) \qquad (IV-\ )$$

or, if ITEM2(J) equals one or three

$$\Sigma^{i,j,l} = N^{j,l} \qquad (IV-\ )$$

The meaning of the symbols are as follows:

$N^{j,l}$ = number density of isotope j in the region ℓ

$\sigma_a^{i,j}$ = Macroscopic absorption cross section of isotope j, ... group i

$\sigma_r^{i,j}$ = Macroscopic removal cross section of isotope j, ... group i

The isotopes included in the summation (IV-1) are ... The coefficient C_{ij}^{kl} and the above absorption ... input data, and are generally group and ... dependent.

III-4 CALCULATION OF THE CROSS SECTIONS

... we would like these diffusion parameters ... recalculation in the calculation of ... the finite difference equation and especially for ... criticality of a reactor. The group constants ... the fuel subregions.

... briefly discussed. The macroscopic cross ... group constants in Chapter IV.

... the index ITD=1, then the diffusion coefficients ... sections, except the scattering matrix, ... subregions DEPCOH. Group constants are ... from ... Thus, they would be defined as:

$$\Sigma_{tr}^{i,j} = \sum_{j=1}^{j_L} N^{j,l} \quad \xi^{i,j,l} \quad \sigma_s^{i,j}$$

Macroscopic transport cross section ... (cm^{-1})

in a similar fashion we can define

$$\Sigma_f^{i,l} = \sum_{j=1}^{NI} N^{j,l} \xi^{i,j,l} \sigma_f^{i,j} \qquad \text{Macroscopic fission cross section } (cm^{-1}) \qquad (IV-50)$$

and

$$\nu\Sigma_f^{i,l} = \sum_{j=1}^{NI} \nu N^{j,l} \xi^{i,j,l} \sigma_f^{i,j} \qquad \text{Macroscopic nu-fission cross section } (cm^{-1}) \qquad (IV-51)$$

and

$$\Sigma_a^{i\to k,l} = \sum_{j=1}^{NI} N^{j,l} \xi^{i,j,l} \sigma_r^{i,j} \qquad \text{Macroscopic removal cross section from group i to k } (cm^{-1}) \qquad (IV-52)$$

and

$$Q^{i,l} = \sum_{j=1}^{NI} N^{j,l} \xi^{i,j,l} \sigma_f^{i,j} e^{i,j} \qquad \text{Macroscopic cross section for energy production } (J/cm) \quad e=3.2 \times 10^{-11} \text{ J} \qquad (IV-53)$$

and

$$\Sigma_{tr}^{i,l} = \sum_{j=1}^{NI} N^{j,l} \xi^{i,j,l} \sigma_{tr}^{i,j} \qquad \text{Macroscopic transport cross section } (cm^{-1}) \qquad (IV-54)$$

and

$$D^{i,l} = \frac{1}{3\sum_{j=1}^{NI} N^{j,l} \xi^{i,j,l} \sigma_{tr}^{j,j}} \qquad \text{Diffusion coefficient (cm)} \qquad (IV-55)$$

The physical interpretations of these symbols are:

NI : total number of isotopes

j : isotope index

i : group index

l : region index

$\sigma_{tr}^{i,j}$: microscopic transport cross section

$\sigma_{a}^{i,j}$: microscopic absorption cross section

$\sigma_{f}^{i,j}$: microscopic fission cross section

ν : average number of neutrons produced per fission

$\epsilon^{i,j}$: energy produced per fission

$\sigma_{r}^{i\ k}$: microscopic removal cross section from group i to k.

GETCON collects the Σa, Σr and $D \times B^2$ which signify the cross section, diffusion coefficient and nu-fission cross section on logical unit 4.

If the variable index IND=2, then the program collects the transport matrix which is also written on logical unit 4.

CHAPTER V

SUBROUTINE CODI

CODI calculates the coefficients of the finite difference equations and prepares the tapes for a strong neutron.

In I we consider how one could attempt to solve the neutron diffusion equation directly by the aid of a digital computer. We saw the advantage of using a computer is its ability to handle large systems of algebraic equations with great speed and accuracy. Our first task is to convert the diffusion equation into a system of algebraic equations more suitable for a digital computer. This is accomplished by "discretizing" each of the terms in the diffusion equation, that is, by replacing the continuous variables by a discrete set of values at a finite number of mesh grid points. The derivatives and integrals in the diffusion equation must also be replaced by finite difference approximations. In this way one obtains a finite set of algebraic equations for the discrete values of the unknown variable which in our case is the neutron flux.

One way of achieving the discretization of the diffusion equation is by using the point scheme. The reactor geometry is represented by a two dimensional mesh the axes of which are the x-axis or r-axis and the y-axis or z-axis. To simplify the description we shall discuss the x-y geometry in detail. It is not difficult to see that the r-z case can be extended to the r-z case. The mesh system is defined as shown in Figure 5.1 by the mesh lines. In this system, each mesh point is given a number. Considering the multigroup neutron diffusion equation

$$-\nabla\cdot D^{i}(x,y)\,\nabla\phi^{i}(x,y)+\Sigma_{t}^{i}(x,y)\,\phi^{i}(x,y)=\frac{\chi^{i}}{\lambda}\sum_{j=1}^{NG}\nu\Sigma_{f}^{j}(x,y)\,\phi^{j}(x,y)+\sum_{\substack{j=1\\ j\neq i}}^{NG}\Sigma_{s}^{j\to i}(x,y)\,\phi^{j}(x,y)$$

The coefficients of the general diffusion equation are $D^{i}(x,y)$, $\nu\Sigma_{f}^{i}(x,y)$ and $\Sigma_{s}^{i\to i}(x,y)$. We assume that these coefficients are constant in each mesh square.

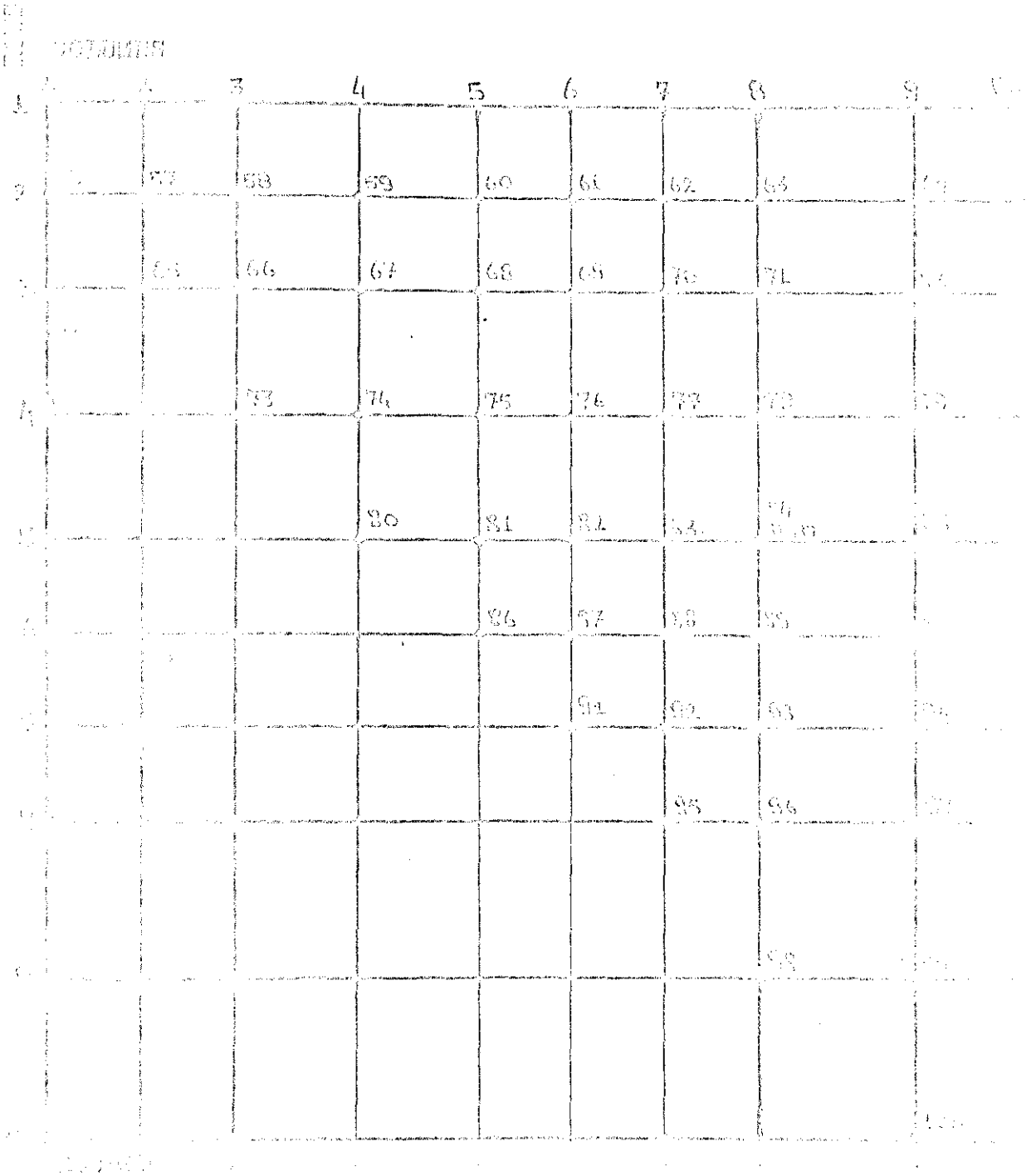


Fig. 7-1. The complete x-y mesh

Let us consider the grid point (m,n) and four adjacent grid points $(m-1,n)$, $(m+1,n)$, $(m,n-1)$ and $(m,n+1)$ as illustrated in Figure V-2. Four rectangular boxes around the point (m,n) are defined by lines passing through the midpoints between the point (m,n) and the neighboring ones. Thus, there are four boundary volumes around the mesh point (m,n). These volumes are labeled 1, 2, 3, and 4 in Figure V-2. Each volume may or may not have different energy boundaries, or different region indices; since for each mesh point is always taken to be mesh points.

Subroutine CODI calculates V_1, V_2, V_3, and V_4 the four volumes indicated in Figure V-2.

$$V_2 = \frac{\Delta x_2 \cdot \Delta y_1}{4}, \quad V_2 = \frac{\Delta x_1 \cdot \Delta y_1}{4}, \quad V_3 = \frac{\Delta x_1 \cdot \Delta y_2}{4}, \quad V_4 = \frac{\Delta x_2 \cdot \Delta y_2}{4}$$

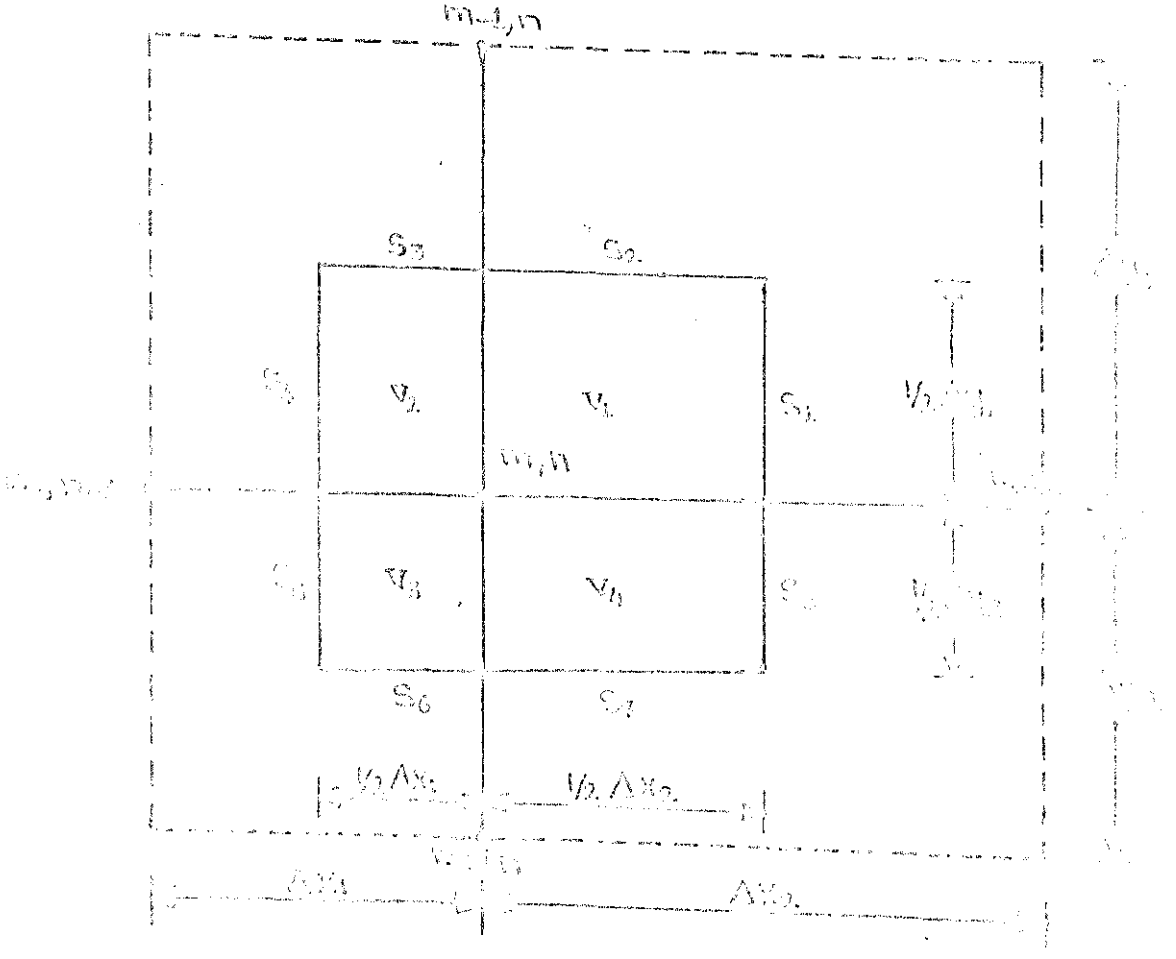


Figure V-2 Part of the mesh shown in detail.

Reactor regions have been described in subprogram [illegible] that the mesh points have already been assigned to different regions via the assignment statements;

IC1 = ICMP(N1)

IC2 = ICMP(N2)

IC3 = ICMP(N3)

IC4 = ICMP(N4)

where N1, N2, N3, and N4 are the mesh point numbers which are located at the left bottom corners of the mesh squares, of which each point number describes a different mesh square.

IC1, IC2, IC3, and IC4 are the region indices. A region may contain one or more mesh squares.

V-A COEFFICIENTS OF THE FINITE DIFFERENCE EQUATIONS

The difference equations are obtained by integrating the [illegible] equation over the four rectangular volumes surrounding the mesh point (m,n)

$$-\int_V \nabla\cdot D^i(x,y)\nabla\phi^i(x,y) + \int_V \Sigma_t^i(x,y)\phi^i(x,y) = \frac{\chi^i}{k}\nu\sum_{j=1}^{NG_2}\int_V \nu\Sigma_f^j(x,y)\phi^j(x,y) + \sum_{\substack{j=1\\ j\neq i}}^{NG_2}\int_V \Sigma_s^{j\to i}(x,y)\phi^j(x,y) \qquad (V-1)$$

We will treat each term separately. The first integral is the [illegible] of the region of integral and $\partial/\partial n$ is the [illegible] to the surface;

$$-\int_V \nabla\cdot D^i(x,y)\nabla\phi^i(x,y)dV = -\int_S D^i(x,y)\nabla\phi^i(x,y)\cdot dS \qquad (V-2)$$

By [illegible] the surface integral of the right side of [illegible], we approximate the derivative by

$$\frac{\phi^i_{m+1,n}-\phi^i_{m,n}}{\Delta x_2} \quad \text{on the surface } S_2 \text{ and } S_3 \qquad (V-3)$$

$$\frac{\phi^i_{m-1,n}-\phi^i_{m,n}}{\Delta x_1} \quad \text{on the surface } S_1 \text{ and } S_3 \qquad (V-4)$$

$$\frac{\phi^i_{m,n-1}-\phi^i_{m,n}}{\Delta x_1} \quad \text{on the surface } S_1 \text{ and } S_3 \qquad (V-5)$$

$$\frac{\partial \phi^i}{\partial y} = \frac{\phi^i_{m+1,n} - \phi^i_{m,n}}{\Delta y_2} \qquad \text{on the surface } S_4 \text{ and } S_2 \qquad (V\text{-}C)$$

The surface integrals along S_1 and S_3, for example, become

$$-\int_{S_1} D^i(x,y)\, \nabla \phi^i(x,y)\, dS = -D^i_1 \frac{\phi^i_{m,n-1} - \phi^i_{m,n}}{\Delta y_1} \cdot \frac{\Delta x_2}{2} - D^i_2 \frac{\phi^i_{m,n-1} - \phi^i_{m,n}}{\Delta y_1}$$

$$= \frac{D^i_1 \Delta x_2 + D^i_2 \Delta x_1}{2 \Delta y_1} \left(\phi^i_{m,n} - \phi^i_{m-1,n} \right) \qquad (V$$

The surface integrals along the other surfaces may be [illegible] calculated similarly;

$$\frac{D^i_1 \Delta y_1 + D^i_2 \Delta y_2}{2 \Delta x_1} \left(\phi^i_{m,n} - \phi^i_{m,n-1} \right) \qquad \text{along } S_4 \text{ and } S_2 \qquad (V$$

$$\frac{D^i_3 \Delta y_3 + D^i_4 \Delta y_2}{2 \Delta x_2} \left(\phi^i_{m,n} - \phi^i_{m+1,n} \right) \qquad \text{along } S_3 \text{ and } S_1 \qquad (V$$

$$\frac{D^i_3 \Delta y_3 + D^i_4 \Delta y_4}{2 \Delta x_2} \left(\phi^i_{m,n} - \phi^i_{m,n+1} \right) \qquad \text{along } S_3 \text{ and } S_4 \qquad (V$$

where D^i_1, D^i_2, D^i_3, and D^i_4 are the diffusion coefficients for regions V_1, V_2, V_3, and V_4 respectively.

The second integral becomes

$$\int_S \Sigma^i_{-t}(x,y)\, \phi^i(x,y)\, dS = \left(\Sigma^i_{-t,1} V_1 + \Sigma^i_{-t,2} V_2 + \Sigma^i_{-t,3} V_3 + \Sigma^i_{-t,4} V_4 \right) \phi^i_{m,n}$$

$$= \sum_{k=1}^{4} \left(\Sigma^i_{-t,k} V_k \right) \phi^i_{m,n}$$

where $\Sigma^i_{-t,k}$ is the value of $\Sigma^i_{-t}(x,y)$ in the volume [illegible] by V_k ($k = 1, 2, 3, 4$). Similarly the third term on the right hand side of equation (V-2) becomes

$$\frac{2\chi^i \nu}{\lambda} \sum_{j=1}^{NG} \int_S \nu \Sigma^j_f(x,y)\, \phi^j(x,y)\, dS = \frac{\chi^i \nu}{\lambda} \sum_{j=1}^{NG} \left(\Sigma^j_{f,1} V_1 + \Sigma^j_{f,2} V_2 + \Sigma^j_{f,3} V_3 + \Sigma^j_{f,4} V_4 \right) \phi^j_{m,n}$$

$$= \frac{\chi^i \nu}{\lambda} \sum_{j=1}^{NG} \sum_{k=1}^{4} \Sigma^j_{f,k} V_k\, \phi^j_{m,n} \qquad (V$$

where Σ^{i}_{Rk} is the value of $\Sigma^{i}_{R}(x,y)$ in the volume region V_k. The second integral on the right side of Equation (V-

$$\sum_{\substack{j=1\\ j\neq i}}^{NG}\int_{S}\Sigma_{R}^{j\to i}(x,y)\phi^{j}(x,y)\,ds = \sum_{\substack{j=1\\ j\neq i}}^{NG}\left(\Sigma_{R1}^{j\to i}\cdot V_1+\Sigma_{R2}^{j\to i}\cdot V_2+\Sigma_{R3}^{j\to i}\cdot V_3+\Sigma_{Rk}^{j\to i}\cdot V_k\right)\phi^{j}_{m,n}$$

$$= \sum_{\substack{j=1\\ j\neq i}}^{NG}\sum_{k=1}^{I_L}\Sigma_{Rk}^{j\to i}\cdot V_k\cdot\phi^{j}_{m,n} \qquad (V-$$

where $\Sigma^{j\to i}_{Rk}$ is the value of $\Sigma^{j\to i}_{R}(x,y)$ in the volume region by V_k.

The last two equations (V-13) and (V-14) constitute the two terms of the diffusion equation. The source terms can be represented as a single term such as $S^{i}_{m,n}$. Thus;

$$S^{i}_{m,n} = \frac{\chi^{i}\nu}{\lambda}\sum_{j=1}^{NG}\sum_{k=1}^{I_L}\Sigma^{j}_{fk}V_k\phi^{j}_{m,n}+\sum_{\substack{j=1\\ j\neq i}}^{NG}\sum_{k=1}^{I_L}\Sigma^{j\to i}_{Rk}\cdot V_k\cdot\phi^{j}_{m,n} \qquad (V-$$

Collecting all the terms together, we obtain the five point diffusion equation;

$$a^{i}_{m,n}\phi^{i}_{m+1,n}+b^{i}_{m,n}\phi^{i}_{m-1,n}+c^{i}_{m,n}\phi^{i}_{m,n+1}+d^{i}_{m,n}\phi^{i}_{m,n-1}+e^{i}_{m,n}\phi^{i}_{m,n} = S^{i}_{m,n}$$

where the coefficient are;

$$e^{i}_{m,n} = -\sum_{k=1}^{I_L}\Sigma^{i}_{Rk}V_k-\left(b^{i}_{m,n}+c^{i}_{m,n}+d^{i}_{m,n}+a^{i}_{m,n}\right)$$

$$a^{i}_{m,n} = -\frac{a^{i}\Delta x_1+D^{i}_{1}\Delta x_2}{2\Delta x_2} \qquad (V-$$

$$d^{i}_{m,n} = -\frac{D^{i}_{1}\Delta x_2+D^{i}_{2}\Delta x_1}{2\Delta x_1} \qquad (V-$$

$$c^{i}_{m,n} = -\frac{D^{i}_{1}\Delta x_1+D^{i}_{2}\Delta x_2}{2\Delta x_2} \qquad (V-$$

$$a^i_{m,n} = -\frac{D^i_2 \Delta y_1 + D^i_1 \Delta y_2}{2\Delta x_1} \qquad (V-29)$$

In the preceding equation, $b_{m,n}$, $c_{m,n}$, $d_{m,n}$, $e_{m,n}$ are negative and $a_{m,n}$ is positive when $D \geq 0$ and $\Sigma^i_{tr} \geq 0$. Notice also that by properties $b^i_{m,n} = d^i_{m,n}$ and $c^i_{m,n} = e^i_{m,n}$.

V-3 FINITE DIFFERENCE EQUATIONS NEAR A BOUNDARY

If the mesh point (m,n) is on an outer boundary, the difference equation is derived by using the boundary condition which is generally expressed as

$$D \frac{\partial}{\partial n} \phi(s) + \gamma(s)\, \phi(s) = 0 \qquad (V-30)$$

where s is the coordinate along the boundary; then

$$\gamma(s) = \frac{\alpha}{D} \qquad (V-31)$$

The boundary condition at the edge of the reactor core is

$$\phi(x,y) = 0 \qquad \text{for} \quad m=1 \quad \text{or} \quad M=IPX \qquad (V-32)$$

$$\phi(x,y) = 0 \qquad \text{for} \quad n=1 \quad \text{or} \quad N=NPX \qquad (V-33)$$

An alternative set of boundary conditions could be;

$$\beta(x,y)\, D(x,y) \frac{\partial \phi(x,y)}{\partial x} + \alpha(x,y)\, \phi(x,y) = 0 \qquad (V-34)$$

$$\beta(x,y)\, D(x,y) \frac{\partial \phi(x,y)}{\partial y} + \alpha(x,y)\, \phi(x,y) = 0 \qquad (V-35)$$

For the particular outer boundary for example, the leakage is zero by the condition in Equation (V-34) if $\beta(x,y)$ is equal to zero for all x,y of the condition in Equation (V-34), then we integrate the diffusion equation

over the volumes v_2 and v_3. The contributions for v_1 and v_4 are zero, because they now don't exist. The contributions of the surfaces S_3, S_4, S_5, and S_6 are the same as before. The surfaces S_1, S_2, S_7, and S_8 don't exist for this boundary point, but we have the new surfaces S_1' and S_8'.

The surface integral for the first term of Equation (V-2) is performed along the surfaces of v_2 and v_3. The derivatives $\partial\phi/\partial(x,y)$ normal to the surfaces S_1' and S_8' are evaluated by Equation (V-22), so that the surface integral along S_1' and S_8' becomes:

$$\int D(x,y)\nabla\phi(x,y)\,dx\,dy = -\int \gamma(x,y)\,\phi(x,y)\,dx\,dy$$

$$= -\left(\frac{\gamma_1^i \Delta y_1}{2} + \frac{\gamma_8^i \Delta y_2}{2}\right)\phi_{m,n} \qquad (V-23)$$

where γ_1^i and γ_8^i are the values of $\gamma(x,y)$ on S_1' and S_8' respectively.

The surface integrals along S_4 and S_5 become:

$$\frac{D_4^i \Delta y_2}{2\Delta x_{-1}}\left(\phi_{m,n}^i - \phi_{m,n-1}^i\right) \qquad (V-24)$$

and along S_3

$$\frac{D_3^i \Delta y_1}{\Delta x_1}\left(\phi_{m,n}^i - \phi_{m-1,n}^i\right) \qquad (V-25)$$

and along S_6

$$\frac{D_6^i \Delta y_2}{2\Delta x_2}\left(\phi_{m,n}^i - \phi_{m+1,n}^i\right) \qquad (V-26)$$

The distribution for v_2 and v_3 are unchanged. Equations (V-2) apply only to v_2 and v_3. The left hand and right side of Equation (V-2) become:

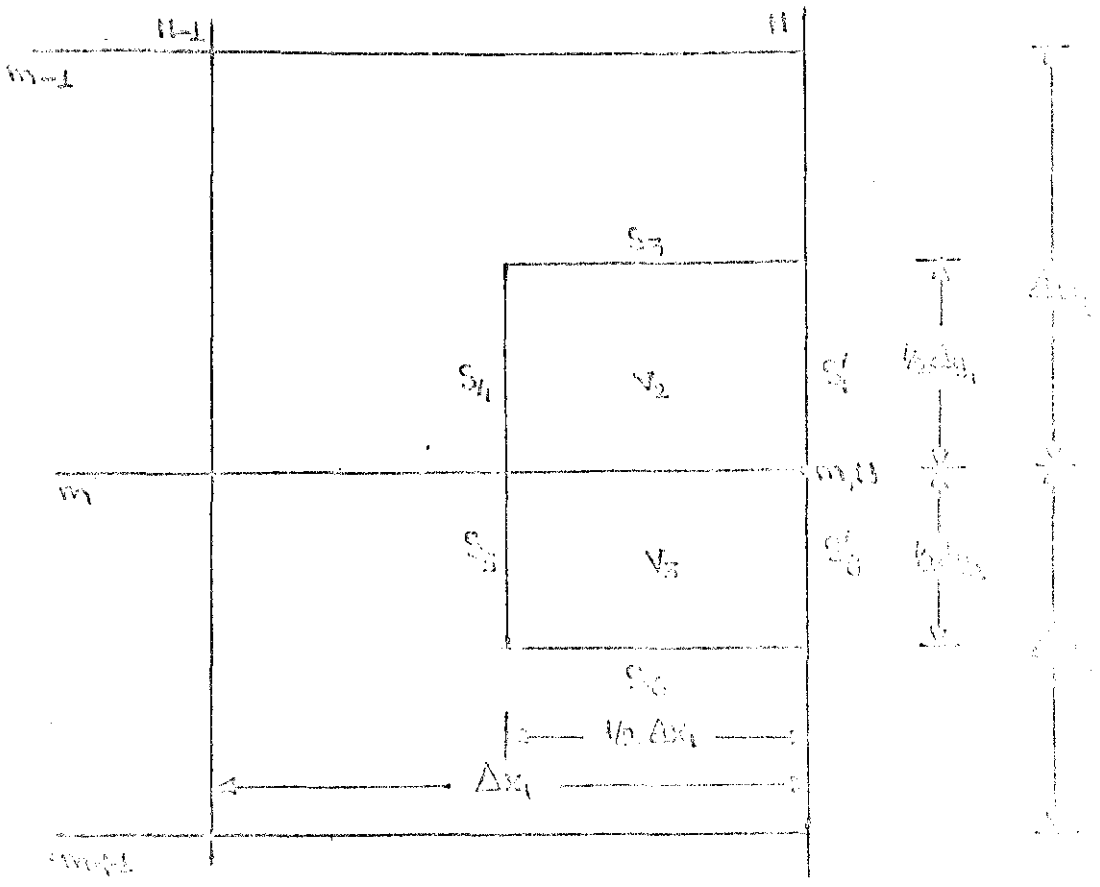


Figure V-3 Area of integration near the outer boundary.

$$\int_{S_1} \Sigma_{t_1}^{i}(x,y)\ \phi(x,y)\,dx\,dy = \left(\Sigma_{t_2}^{i}\cdot V_2 + \Sigma_{t_3}^{i}\cdot V_3\right)\phi_{m,n}^{i} \qquad (V-\ )$$

$$\frac{\chi_m^i \nu}{\lambda}\int_{S_1}\Sigma_f^i(x,y)\ \phi^j(x,y)\,dx\,dy = \frac{\chi_m^i \nu}{\lambda}\sum_{j=1}^{nG}\left(\Sigma_{f2}^{j}\cdot V_2 + \Sigma_{f3}^{j}\cdot V_3\right)\phi_{m,n}^{j} \qquad (V-\ )$$

$$\sum_{\substack{j=1\\ j\neq i}}^{nG}\Sigma_{s_0}^{j\to i}(x,y)\ \phi^j(x,y)\,dx\,dy = \sum_{\substack{j=1\\ j\neq i}}^{nG}\left(\Sigma_{R2}^{j\to i}\cdot V_2 + \Sigma_{R3}^{j\to i}\cdot V_3\right)\phi_{m,n}^{j} \qquad (V-\ )$$

The source terms can be represented as a single term such as $Q_{m,n}^{i}$. Then

$$S_{m,n}^{i} = \left[\frac{\chi_m^i \nu}{\lambda} - \sum_{j=1}^{nG}\left(\Sigma_{f2}^{j}\cdot V_2 + \Sigma_{f3}^{j}\cdot V_3\right) + \sum_{\substack{j=1\\ j\neq i}}^{nG}\left(\Sigma_{R2}^{j\to i}\cdot V_2 + \Sigma_{R3}^{j\to i}\cdot V_3\right)\right]\phi_{m,n}^{i} \qquad (V-\ )$$

Collecting all the terms, the difference equation is expressed by Equation (V-16) with the coefficients as;

$$c^i_{m,n} = \Sigma_{t2}\, v_2 + \Sigma_{t3}\, v_3 - \left(b^i_{m,n} + c^i_{m,n} + d^i_{m,n} + e^i_{m,n} + \frac{\gamma^i_{m,n}\Delta x_1 + \gamma^i_{m,n}\Delta y_1}{2}\right) v_1$$

$$b^i_{m,n} = -\frac{D^i_3 \Delta x_1}{2\Delta y_2}$$

$$d^i_{m,n} = 0$$

$$e^i_{m,n} = -\frac{D^i_3 \Delta x_1}{2\Delta y_1}$$

$$c^i_{m,n} = -\frac{D^i_2 \Delta y_1 + D^i_2 \Delta y_2}{2\Delta x_1}$$

The difference equations for Equation (V-2), in terms of other two dimensional coordinate system, r-z or z-θ, can be obtained similarly by evaluating the volume and surface of the cell properly.

CHAPTER VI

SOLUTION OF THE FINITE DIFFERENCE EQUATIONS

We have now finished the discussion of the setting up of the finite difference equations. The next problem is to solve these equations bearing in mind that a typical problem will have between 1500 and 10000 spatial mesh points in each energy group. Our first task is to cast the set of equations into matrix form. For the sake of later discussion, it will be convenient to write Equation (V-16) in the matrix form.

$$A = \begin{bmatrix} a_{11} & b_{11} & & & d_{11} & & & & \\ c_{21} & a_{21} & b_{21} & & & d_{21} & & & \\ & c_{31} & a_{31} & b_{31} & & & d_{31} & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & c_{m1} & a_{m1} & b_{m1} & & \\ c_{12} & & & & & c_{12} & a_{12} & b_{12} & \\ & c_{22} & & & & & c_{22} & a_{22} & b_{22} \\ & & & & & & & & \end{bmatrix}$$

The configuration of A depends on how the elements of the vector $\vec{\phi}$ correspond to $\phi_{n,m}$.

Let

$$\phi = \begin{bmatrix} \phi^i_{1,1} \\ \phi^i_{2,1} \\ \vdots \\ \phi^i_{M,1} \\ \phi^i_{1,2} \\ \phi^i_{2,2} \\ \vdots \\ \phi^i_{M,2} \\ \phi^i_{1,3} \\ \phi^i_{2,3} \\ \vdots \\ \phi^i_{M,N} \end{bmatrix} \quad \text{and} \quad S = \begin{bmatrix} S^i_{1,1} \\ S^i_{2,1} \\ \vdots \\ S^i_{M,1} \\ S^i_{1,2} \\ S^i_{2,2} \\ \vdots \\ S^i_{M,2} \\ S^i_{1,3} \\ S^i_{2,3} \\ \vdots \\ S^i_{M,N} \end{bmatrix} \qquad (VI.-1)$$

where i is the group index.

It is apparent that the general structure of the finite difference multigroup diffusion equations may be expressed in the matrix form as

$$A\,\phi = S, \qquad (VI.-2)$$

In matrix notation the elements of a column vector $\phi_{P,1}$ are denoted by $\phi_1, \phi_2, \ldots$ and those of the coefficient matrix A by $A_{i,j}$. Thus

$$\phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_{P-1} \\ \phi_P \end{bmatrix} \qquad A = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,P-1} & A_{1,P} \\ A_{2,1} & & & & A_{2,P} \\ \vdots & & & & \vdots \\ A_{P-1,1} & & & & A_{P-1,P} \\ A_{P,1} & \cdots & & A_{P,P-1} & A_{P,P} \end{bmatrix} \qquad (VI.-3)$$

Sometimes, it is convenient to think of the elements of the vector $\phi_1, \phi_2, \ldots\ldots$ etc. as belonging to a two dimensional mesh. We thus have

$$
\begin{aligned}
\phi_1 &= \phi_{1,1} \\
\phi_2 &= \phi_{2,1} \\
\phi_3 &= \phi_{3,1} \\
&\vdots \\
\phi_M &= \phi_{M,1} \\
\phi_{M+1} &= \phi_{1,2} \\
\phi_{M+2} &= \phi_{2,2} \\
&\vdots \\
\phi_{2M} &= \phi_{M-1,N} \\
\phi_P &= \phi_{M,N}
\end{aligned}
\qquad\qquad
\begin{aligned}
A_{1,1} &= a_{1,1} \\
A_{1,2} &= b_{1,1} \\
A_{1,3} &= 0 \\
&\vdots \\
A_{1,N} &= d_{1,1} \\
A_{2,1} &= c_{2,1} \\
A_{2,2} &= a_{2,1} \\
&\vdots \\
A_{M+1,M+1} &= a_{1,2} \\
&\vdots \\
A_{P,P} &= a_{M,N}
\end{aligned}
$$

from which it is obvious that the dimension of the floor is $P \times P$. The matrix A has certain special properties such as

a. A is symmetric.

b. The diagonal elements are positive. The off-diagonal elements are zero or negative.

c. The absolute value of the diagonal term in any row is greater than the sum of the absolute values of the off-diagonal elements of that row. It is this property that gives rise to zeros. The difference between the diagonal and the sum of the off-diagonal ones is denoted by $h_{m,n}$ and is defined as

$$h_{m,n} = a_{m,n} - \left(b_{m,n} + c_{m,n} + d_{m,n} + e_{m,n}\right) \qquad \text{(VI-5)}$$

The terms $c_{m,n}$, $d_{m,n}$, and $e_{m,n}$ have been given in (VI-4) as being either positive or zero. For such points as $\phi_{m,n}$, the difference between diagonal and off-diagonal will still positive. For example, for the boundary point $\phi_{1,1}$ the difference is;

$$d^i_{m,N} = a^i_{m,N} - (b^i_{m,N} + c^i_{m,N} + e^i_{m,N}) \qquad \text{(VI-6)}$$

Consider the mesh system consisting of nine grid points as shown in Figure VI-2(a). If we array ϕ_{mn} in the sequence shown in Figure VI-1(b), then Equation (VI-3) becomes:

$$\begin{bmatrix} a_{11} & b_{11} & 0 & d_{11} & 0 & 0 & 0 & 0 & 0 \\ c_{21} & a_{21} & b_{21} & 0 & d_{21} & 0 & 0 & 0 & 0 \\ 0 & c_{31} & a_{31} & 0 & 0 & d_{31} & 0 & 0 & 0 \\ e_{12} & 0 & 0 & a_{12} & b_{12} & 0 & d_{12} & 0 & 0 \\ 0 & e_{22} & 0 & c_{22} & a_{22} & b_{22} & 0 & d_{22} & 0 \\ 0 & 0 & e_{32} & 0 & c_{32} & a_{32} & 0 & 0 & d_{32} \\ 0 & 0 & 0 & e_{13} & 0 & 0 & a_{13} & b_{13} & 0 \\ 0 & 0 & 0 & 0 & e_{23} & 0 & c_{23} & a_{23} & b_{23} \\ 0 & 0 & 0 & 0 & 0 & e_{33} & 0 & c_{33} & a_{33} \end{bmatrix} \begin{bmatrix} \phi_{11} \\ \phi_{21} \\ \phi_{31} \\ \phi_{12} \\ \phi_{22} \\ \phi_{32} \\ \phi_{13} \\ \phi_{23} \\ \phi_{33} \end{bmatrix} = \begin{bmatrix} s_{11} \\ s_{21} \\ s_{31} \\ s_{12} \\ s_{22} \\ s_{32} \\ s_{13} \\ s_{23} \\ s_{33} \end{bmatrix} \qquad \text{(VI-7)}$$

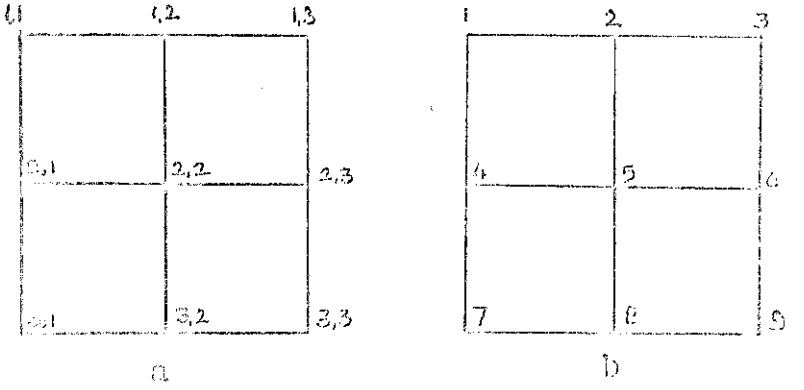


Figure VI-2

Since this Equation (VI-7) is a pentadiagonal matrix, it would [illegible] solution of this matrix equation [illegible] Instead, we will employ an iterative method to converge to the exact solution [illegible]

iterative solution is convergent if the spectral radius of the iterative matrix is less than unity. Of course, it is [illegible] very difficult or impossible to know all the eigenvalues of a matrix if the order of matrix is large. There are, however, certain theorems that give sufficient conditions to ensure eigenvalues less than unity. A proof of the theorems and a few of the [illegible] properties, related to iterative convergence, can be found in [illegible] textbooks on matrix theory, for example, Householder (3) and Varga (4). In fact Equation (VI-3) has various favorable properties for iterative relaxation methods.

The following iterative schemes are well known

1. Point Jacobi iterative method.
2. Line Jacobi iterative method.
3. Gauss-Seidel iterative method.
4. Alternating direction implicit method.
5. Successive over relaxation method.
6. Cyclic Chebyshev semi iterative method.

VI-A DETERMINATION OF THE ACCELERATION PARAMETERS FOR HIGHER ITERATION

We now return to the problem of solving Equation (VI-2). [illegible] we illustrate the basic idea with a simple example. Suppose we wish to invert a matrix A, that is, we wish to solve

$$A\phi = S \tag{VI-4}$$

The linear iteration procedure is set up to obtain a [illegible] solution of ϕ. Successive over-relaxation may be [illegible] as a linear iteration procedure. To find [illegible] to be the diagonal and off-diagonal elements.

$$A = D - L - U \tag{VI-5}$$

$$\begin{bmatrix} \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \\ \end{bmatrix} - \begin{bmatrix} \\ \\ \end{bmatrix} - \begin{bmatrix} \\ \\ \end{bmatrix}$$

The spectral radius of a matrix A is the number $\rho(A) = \max |\lambda_i|$, where λ_i is an eigenvalue of A. It can be shown that $\rho(A) \leq \|A\|$, where the spectral radius $\rho(A)$ of a matrix can not exceed the value of its norm.

where D is the diagonal matrix of order P,
L is the lower triangular matrix with null diagonal elements,
U is the upper triangular matrix with null diagonal elements.

The Gauss-Seidel iterative method (4) is then defined by

$$D\,\phi^{(t+1)} = L\,\phi^{(t+1)} + U\,\phi^{t} + S \qquad \text{(VI-10)}$$

or

$$(D-L)\,\phi^{(t+1)} = U\,\phi^{t} + S \qquad \text{(VI-11)}$$

giving

$$\phi^{(t+1)} = (D-L)^{-1}\,U\,\phi^{(t)} + (D-L)^{-1}\,S \qquad \text{(VI-12)}$$

The matrix "$(D-L)^{-1}\,U$" is called the Gauss-Seidel iteration matrix associated with the matrix A.

It is possible to accelerate the convergence of the Gauss-Seidel scheme even further by introducing an acceleration process which yields the iterative flux estimate. This procedure is known as the Successive Overrelaxation (SOR) method. In the SOR method the displacement vector is multiplied by that in the Gauss-Seidel method, where w is the acceleration parameter and is a real number. Hence, by Equation (VI-10) the SOR iteration is defined by

$$D\,\phi^{(t+1)} = \phi^{(t)} + w\left[L\,\phi^{(t+1)} + U\,\phi^{t} + S - \phi^{(t)}\right] \qquad \text{(VI-13)}$$

Here the acceleration parameter w ranges between 1 and 2. If w is set equal to 1, we return to the Gauss-Seidel method in which no acceleration is used. Equation (VI-13) can be written as

$$\phi^{(t+1)} = (D-wL)^{-1}\left[wU-(w-1)D\right]\phi^{t} + (D-wL)^{-1}\,wS \qquad \text{(VI-14)}$$

The convergence rate of the SOR method is dependent on the value of w. However, the proper choice of w is problem-dependent when the given problem is intrinsically slowly convergent. If the solution method employs the acceleration process for

repeatedly, it is worthwhile to develop a subprogram to calculate the optimal w. For this reason, subprogram VTM36 is provided.

Various methods of computing the accelerating parameter w has been investigated by D.A.Carre (5) who considered a problem for which the best value of w, denoted by w_{opt}, equals 1.95 and gives a rate of convergence forty times greater than that obtained by using w=1 (Gauss-Seidel).

Unfortunately there are no simple formula for calculating w_{opt}, so its value must be estimated. This depends upon estimates of either the spectral radius $\rho(j)$ of the corresponding Jacobi iteration matrix (L+U), or the spectral radius $\rho(G)$ of the Gauss-Seidel iteration matrix $(D-L)^{-1}U$. Assuming that the matrix of the finite difference equation possesses the Property A and is consistently ordered (6), then it can be proved that

$$\rho(G) = \rho^2(j) \qquad \text{(VT-...)}$$

$$w_{opt} = \frac{2}{1+\sqrt{1-\rho(G)}} \qquad \text{(VT-...)}$$

Carre, reference 5, and Varga, give several methods for estimating $\rho(G)$ and $\rho(j)$.

One such method calculates a large set of successive approximations $\phi^{(1)}$, $\phi^{(2)}$, ... $\phi^{(k)}$ to the solution of the Poisson equations by Gauss-Seidel iterations and then estimates $\rho(G)$ from

$$\rho(G) = \lim_{k\to\infty} \frac{\| d^{(k+1)} \|}{\| d^{k} \|} \qquad \text{(VT-...)}$$

where $d^{(k)} = \phi^{(k+1)} - \phi^{(k)}$ and $\| d^{(k+1)} \|$, the norm of $d^{(k+1)}$, is defined by

$$\| d^{(k+1)} \| = |\phi^{(k+1)} - \phi^{k}| + |\phi^{(k+1)} - \phi^{k}| + \ldots + |\phi^{(k+1)} - \phi^{k}| \qquad \text{(VT-...)}$$

or

$$\| d^{(k+1)} \| = \text{maximum of } |\phi_i^{(k+1)} - \phi_i^{(k)}| \quad i=1,2,\ldots p \qquad \text{(VT-...)}$$

or

$$\|a^{(t+1)}\| = \left[\left(\phi_1^{(t+1)} - \phi_1^{(t)} \right)^2 + \left(\phi_2^{(t+1)} - \phi_2^{(t)} \right)^2 + \cdots + \left(\phi_p^{(t+1)} - \phi_p^{(t)} \right)^2 \right]^{1/2} \qquad \text{(VII-}\cdots\text{)}$$

If the spectral radii, $\rho(G)=\mathrm{AMD}(IG)$, are initially given as input then these are used to determine the optimum overrelaxation parameters w_{opt} to be used in the acceleration scheme.

If $\rho(G)=\mathrm{AMD}(IG)$ are not provided then ROMI, and ROMA (minimum and maximum spectral radii) are estimated by VIII-36 and using these values in an extrapolation procedure ROMI (average spectral radii) are obtained and assigned as the values of $\rho(G)$, MAXIT which are then used to find w through the function $\mathrm{FOG}(\rho(G))$

$$\mathrm{FOG}(\rho(G)) = \frac{2}{1+\sqrt{1-\rho(G)}} \qquad \text{(VII-}\cdots\text{)}$$

If any one of the estimated values for ROMI, ROMA and ROMI by VIII-36 is greater than one, then VIII-36 makes a new estimate for this until they all are less than or equal to one. The program calculates maxima, minima and average overrelaxation factors by using the function

$$\mathrm{FOG}(x) = \frac{2}{1+\sqrt{1-x}} \qquad \text{(VII-}\cdots\text{)}$$

$$\mathrm{ROMI} = \rho_{max}(G),\ \mathrm{ROMA} = \rho_{min}(G),\ \mathrm{ROMI} = \rho_{ave}(G)$$

$$w_{max} = \frac{2}{1+\sqrt{1-\rho_{max}(G)}} \qquad \text{(VII-}\cdots\text{)}$$

By the same way w_{min} and w_{opt} are calculated as;

$$w_{min} = \frac{2}{1+\sqrt{1-\rho_{min}(G)}} \qquad \text{(VII-}\cdots\text{)}$$

$$w_{opt} = \frac{2}{1+\sqrt{1-\rho_{opt}(G)}} \qquad \text{(VII-}\cdots\text{)}$$

after which ZT is obtained from

$$ZT = \frac{\omega_{max} - \omega_{min}}{2 - \omega_{opt}} \qquad (VI-1)$$

If ZT ≤ 0.2 then calculation of the overrelaxation factors is completed and these values are written as output.

For the application of the Chebyshev polynomials to the overrelaxation coefficient, it is assumed that the eigenvalues of the iterative process are real. First the number of extrapolation factors to be found is determined and then an array of factors is computed as follows;

$$\omega_1 = 1 \qquad (VI-2)$$

$$\omega_2 = \frac{2}{2 - \rho_{ave}(G)} \qquad (VI-3)$$

$$\omega_n = \frac{1}{1 - \rho_{ave}(G) \cdot \omega_{n-1}} \qquad \text{for } n > 2 \qquad (VI-4)$$

A separate set of Chebyshev extrapolation parameters is calculated by the program for each group. Thus we obtain the overrelaxation parameters required for the inner iterations.

VI-2 STRATEGIES FOR SOLVING THE FINITE DIFFERENCE MULTIGROUP DIFFUSION EQUATIONS

If we recall the general discussion of finite difference representations of the neutron diffusion equations given in Section V.2 it is apparent that the general structure of the finite difference multigroup diffusion equations takes the form;

$$a^i_{m,n}\,\phi^i_{m,n} + b^i_{m,n}\,\phi^i_{m+1,n} + c^i_{m,n}\,\phi^i_{m-1,n} + d^i_{m,n}\,\phi^i_{m,n+1} +$$

$$e^i_{m,n}\,\phi^i_{m,n-1} = R^i_{m,n} \qquad (VI-5)$$

Notice that in addition to the coupling to different energy group fluxes at a given mesh point due to the fission source and scattering the finite difference equation is coupled as well to the flux at adjacent spatial mesh point because of the effect of spatial diffusion.

If we denote the number of spatial mesh points by I, I, I and the number of groups by NG, then Equation (VI-73) represents a set of I·I·I·NG simultaneous linear algebraic equations. Since this normalizes the flux at one energy group-space mesh point, the overall normalization of the flux is arbitrary in a criticality calculation. Hence, we have I·I·I equations available to determine the (I-1)·I·I·NG fluxes and the multiplication eigenvalue. Therefore, it is convenient to rewrite this set of equations as a matrix eigenvalue problem

$$A\phi = \frac{1}{\lambda} F\phi \qquad \text{(VI-74)}$$

There are two problems to be resolved;

1. Often the matrix A is so large that it is very difficult to invert it so an approximate method of solution must be introduced leading to inner iterations.

2. The vector S is, of course, unknown since S is directly determined by ϕ. The most commonly used method for solving for ϕ (and hence S) is the power iteration method.

The outer iteration is primarily concerned with obtaining the eigenvalue λ. The power method is an iteration scheme for obtaining the largest eigenvalue λ which is the multiplication factor. The multiplication factor is the ratio of two successive iterations which can be thought of as a ratio of the fission source at one iteration step t to the value of the same quantity at the previous iteration step (t-1).

The iteration scheme proceeds as follows:

define a vector

$$\Psi = \frac{1}{\lambda} F\phi = \frac{1}{\lambda} S \qquad \text{(VI-75)}$$

where

$$S = F\phi \qquad \text{(VI-76)}$$

which is called the source vector. The iteration is defined by the relation

$$A\phi^{(t)} = \psi^{(t-1)} \qquad \text{(VI-30)}$$

so that from Equation (VI-31), we have

$$S^{(t)} = F\phi^{(t)} \qquad \text{(VI-31)}$$

Obtain the iteration source by using Equation (VI-30)

$$\psi^{(t)} = \frac{1}{\lambda^{(t)}} S^{(t)} \qquad \text{(VI-32)}$$

After that, obtain new flux vector by using Equation (VI-14)

$$\phi^{t+1} = (D-wL)^{-1} \left[wU-(w-1)D\right] \phi^{t} + (D-wL)^{-1} wS^{(t)}$$

Note that in inner iterations $S^{(t)}$ denotes what $\psi^{(t)}$ denotes in outer iterations and multiplying by $F^{(t)T}$ we obtain

$$\lambda^{(t)} = \frac{S^{(t)T} \cdot S^{(t)}}{S^{(t)T} \cdot \psi^{(t)}} \qquad \text{(VI-33)}$$

Let us now review the general iterative strategy for solving this eigenvalue problem.

1. One first makes an initial guess of the flux vector $\phi^{(0)}$ and multiplication eigenvalue $\lambda^{(0)}$.

2. Using Equation (VI-33) estimate, the source vector

$$S^{(0)} = F\phi^{(0)} \qquad \text{(VI-34)}$$

and also using Equation (VI-30) estimate the $\psi^{(0)}$

$$\psi^{(o)} = \frac{1}{\lambda^{(o)}} S^{(o)} \qquad \text{(VI-39)}$$

3. At this point one proceeds to solve the inhomogeneous matrix Equation

$$A\phi^{(t)} = \frac{1}{\lambda^{(t-1)}} S^{(t-1)} \qquad \text{(VI-40)}$$

for the next flux iterate ϕ^t. This solution involves a number of substeps.

a. One solves the inhomogeneous diffusion Equation characterizing each of the energy groups.

$$A\phi_i^t = \frac{1}{\lambda^{(t-1)}} S_i^{(t-1)} \qquad \text{(VI-40)}$$

by solving first for the highest energy group, i=1 and using ϕ_1^t to solve for $\phi_2^{(t)}$, and so on, solving successively down the groups.

b. Of course, solving even the inhomogeneous diffusion equation for a single group is no trivial matter for multidimensional problems, iterative techniques will be necessary such as SOR which was discussed in section VI-A. Inner iterations will use the previous flux estimate $\phi_i^{(t-1)}$ as their first guess in solving Equation (VI-40). It should be mentioned that a number of schemes have been proposed for coupling such inner iterations to the outer iterations in order to accelerate convergence.

4. Having obtained the flux estimate $\phi^{(t)}$, source vector is estimated by Equation (VI-33)

$$S^{(t)} = F\phi^{(t)} \qquad \text{(VI-41)}$$

5. Having obtained the source estimate S^t, one can now

determine the new estimate for the multiplication factor by using Equation (VI-36)

$$\lambda^{(t)} = \frac{S^{(t)T} \cdot S^{t}}{S^{(t)T} \cdot \Psi^{(t-1)}} \qquad \text{(VI-42)}$$

6. Calculate a new Ψ using Equation (VI-30)

$$\Psi^{(t)} = \frac{1}{\lambda^{(t)}} S^{(t)} \qquad \text{(VI-43)}$$

7. At this point one tests the outer iteration for convergence by the criterion:

$$\left| \frac{\lambda^{(t)} - \lambda^{(t-1)}}{\lambda^{(t)}} \right| < 10^{-1} \eta \qquad \text{(VI-44)}$$

where η is the convergence criterion for the criticality search. If the changes in $\lambda^{(t)}$ are sufficiently small, one assumes that convergence has been achieved and the iterative procedure is ended. If not, then a new source is calculated and the iteration continues, as a repetition of the steps outlined above.

CHAPTER-VII

NORMALIZATION FACTOR AND POWER PROFILES

VII-A SUBROUTINE NORMA

This routine evaluates the region average fluxes, performs a power integration and calculates the flux normalization factor. Normalization factor is computed by dividing the total reactor power for the time step under consideration, which is an input data by the total amount of energy production rate computed by the unnormalized fluxes. The latter is computed by NORMA. Through the use of the data generated for each energy group and stored in the magnetic tape file by LEPRIC. As was explained in SHRCON, this data, including microscopic cross sections, is used to find the self shielding factors and then the macroscopic cross sections.

Total energy production rate in the reactor resulting from unnormalized fluxes is computed as follows. Total energy production rate is here denoted by TOT.

$$TOT = \sum_{IG=1}^{NG} \sum_{L=1}^{NREG} \Sigma_f(L,IG)\ e.\ \phi(L,IG) \qquad (VII-1)$$

where

IG = group index

L = region index

$\Sigma_f(L,IG)$ = macroscopic fission cross section in region L.

e = energy production per fission ($3.2\ 10^{-11}$ joules)

$\phi(L,IG)$ = volume weighted region flux in group IG.

$\Sigma_f(L,IG)$, being a part of macroscopic cross sections, is computed in SHRCON via the use of microscopic data and self shielding factors, e (energy production per fission) is a constant, We will now explain how to calculate, $\phi(L,IG)$, the volume weighted region flux in group IG.

The reactor is divided into regions, in each of which, the program considers an average burnup, that is, constant burnup, average isotopic number densities and macroscopic cross sections to a given region. Also each region consists of a mesh grid.

mesh is represented by a number which is called the mesh number or mesh point number. There may be at most four volume elements around a mesh point. Each volume is assigned to a different mesh point as illustrated in Figure VII-1. Also, each mesh point may

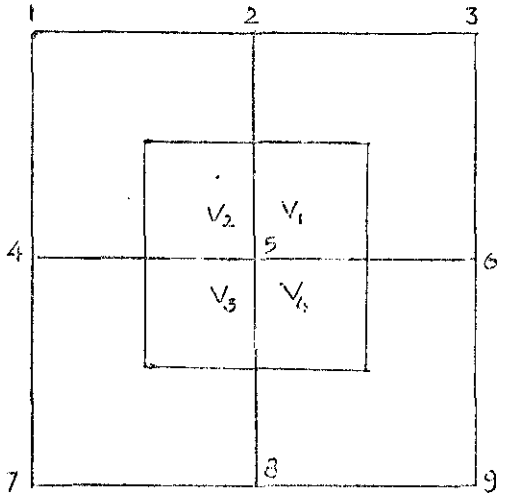


Figure VII-1

belong to a different region. Group constants are the same for all rectangular meshes belonging to a given region. Thus, it will be sufficient to give an example for only one mesh point. If a mesh point is on the boundary then the respective boundary condition is taken into account.

Let us suppose that a mesh point is not on a boundary. In order to compute the quantities needed for say, the mesh point number 5 (see Figure VII-1). Program Sixty determines the neighboring mesh points which are 4, 7, and 8. Each mesh point is known to belong to a specified region. After that, mesh intervals for points 5, 4, 7 and 8 are evaluated and such volumes as those around the point 5 are calculated by the following scheme.

Distances between rows and columns are called mesh spacing lengths, and they are given as input. In the x direction, it is Δx and in the y direction, Δy. Each volume is

$$XYJ = \Delta x . \Delta y \qquad \text{(VII-1)}$$

Now, one can calculate an average point flux from the mesh fluxes read in the logical unit number 9. Calculation of a volume weighted average point flux involves four neighbouring fluxes, in the form;

$$\Psi(L,IG)=\frac{1}{4}\Delta x\cdot\Delta y\left[VET4(5)+VET4(4)+VET4(7)+VET4(8)\right] \qquad (VII-3)$$

This routine is repeated for each mesh point. Along this routine, fluxes belonging to the same region are summed up each time;

$$\phi(L,IG)=\sum_{\ell=1}^{i}\Psi(L,IG) \qquad (VII-4)$$

where ℓ is the mesh point belonging to region L. Thus we obtain the volume weighted region flux for group IG.

If the mesh point under investigation is on a boundary then there would be leakage from this boundary. For example, the top side of the reactor forms a boundary line and if the boundary condition indicator, BCOH(IG,1), is less than zero here the zero flux condition is obtained, in which case leakage from the top side of the reactor is

$$XLEK(IG,1)=D(L,IG)\cdot\frac{VET4(N2)+VET4(N4)-\left[VET4(N1)+VET4(N3)\right]}{\Delta y}\cdot\Delta x \qquad (VII-5)$$

where

N1, N2, N3, and N4 are the mesh point numbers.

Leakage from the other possible boundary sides of the box can be obtained in the same way. At the bottom of the box;

$$XLEK(IG,3)=D(L,IG)\cdot\frac{VET4(N1)+VET4(N2)-\left[VET4(N3)+VET4(N4)\right]}{\Delta y}\cdot\frac{\Delta x}{2}$$

At the left side of the reactor

$$XLSK(IG,2)=D(L,IG)\cdot\frac{VNT4(N2)+VNT4(N4)-\left[VNT4(N1)+VNT4(N3)\right]}{\Delta x}\cdot\frac{\Delta y}{2}$$

(VII-7)

At the right side of the reactor

$$XLRK(IG,4)=D(L,IG)\cdot\frac{VNT4(N1)+VNT4(N3)-\left[VNT4(N2)+VNT4(N4)\right]}{\Delta x}\cdot\frac{\Delta y}{2}$$

We can now calculate the total neutron production which is denoted by FNOR, in the whole reactor

$$FNOR=\sum_{IG=1}^{NG}\sum_{L=1}^{NREG}\nu\cdot\Sigma_f(L,IG)\phi(L,IG) \qquad (VII-9)$$

and total energy production in the whole reactor

$$TOT=\sum_{IG=1}^{NG}\sum_{L=1}^{NREG}e(IG)\,\Sigma_f(L,IG)\phi(L,IG) \qquad (VII-10)$$

For the calculation of the normalization factor, reactor power for the given time step is divided by TOT

$$TOT=\frac{XT}{TOT} \qquad (VII-11)$$

where

XT is given as input and TOT is calculated.

The following calculations are then made by TOTA with the normalization factor, TOT.

Leakage from the reactor boundaries;

$$XLEK(IG,K) = XLEK(IG,K).TOT \qquad (VII-12)$$

Actual neutron production $NOR = \frac{1}{\lambda} NOR.TOT$ (VII-13)

Integrated actual power for region L;

$$ASS(L) = \sum_{IG=1}^{NG} \Sigma_f(L,IG).\phi(L,IG).e(IG).TOT \qquad (VII-14)$$

Integrated actual power for the reactor as a whole;

$$XASS = \sum_{L=1}^{NREG} ASS(L) \qquad (VII-15)$$

Integrated actual source for region L;

$$CPROD(L) = \frac{TOT \sum_{IG=1}^{NG} \nu \Sigma_f(L,IG).\phi(L,IG)}{\lambda} \qquad (VII-16)$$

Integrated actual volume flux for region L and group IG;

$$FF(L,IG) = TOT.\phi(L,IG) \qquad (VII-17)$$

There is no energy generation in some regions of the reactor and therefore, the actual reactor volume is greater than the effective volume.

For the calculation of the actual power density it is necessary to have the effective volume of the reactor. It is hereby denoted by VOLEA;

$$VOLEA = \sum_{\substack{L=1 \\ L \neq NUML}}^{NGRNG} VOL(L) \qquad (VII-19)$$

where

NUML : number of regions in which there is no source generation

VOL(L) : volume of the region L

Actual power density

$$XY = \frac{XASS}{VOLEA} \qquad (VII-20)$$

Average power density in region L; PDL=ASS(L)/VOL(L)

Average source density for region L; SSC=CHSOR(L)/VOL(L)

Form factor that will be helpful in constructing the power profile;

$$XYASS(L) = \frac{PDL}{XY} \qquad (VII-20)$$

VII-3 SUBROUTINE OUTPUT

The goal of this subprogram is to determine the neutron balance. For this reason, OUTPUT calculates the loss terms in the reactor by making use of the group constants read in from logical unit number 4.

The loss terms include absorption, removal and leakage. They are calculated separately in each region for the group G, NL

absorption term is here denoted by ABSINT(IG)

$$\text{ABSINT}(IG)=\sum_{L=1}^{NREG}\Sigma_a(L,IG)\cdot\phi(L,IG) \qquad \text{(VII-61)}$$

The removal term is

$$\text{REMT}(IG)=\sum_{L=1}^{NREG}\Sigma_r(L,IG)\cdot\phi(L,IG) \qquad \text{(VII-62)}$$

Transverse leakage

$$\text{TRLEK}(IG)=\sum_{L=1}^{NREG}D(L,IG)B^2(L,IG)\cdot\phi(L,IG) \qquad \text{(VII-63)}$$

leakage from the reactor boundaries have been obtained in [illegible]. The source term includes sources due to fission and on the collision.

Fission source

$$\text{FSINT}(IG)=\frac{\nu}{\lambda}\sum_{L=1}^{NREG}\Sigma_f(L,IG)\cdot\phi(L,IG) \qquad \text{(VII-64)}$$

Scattering collision source or removal source;

$$\text{SCSOR}(IG)=\sum_{L=1}^{NREG}\sum_{\substack{K=1\\K=IG}}^{NG}\Sigma_R(L,K)\cdot\phi(L,K) \qquad \text{(VII-65)}$$

The energy production in a reactor due to flux in group IG is calculated by the OUTPUT and is represented by QFA(IG)

$$OGA(IG)=\sum_{I=1}^{IREG}\nu\cdot a(IG)\,\Sigma_f(I,IG)\phi(I,IG) \qquad (VII-65)$$

Losses due to absorption, removal and transverse leakage is denoted by ABSINT(IG)

$$ABSINT(IG)=ABSINT(IG)+REMINT(IG)+TRANSV(IG) \qquad (VII-67)$$

Total losses in the reactor denoted by XE2 is;

$$XE2=\sum_{IG=1}^{NG}\left[ABSINT(IG)+\sum_{K=1}^{4}XLEK(IG,K)\right] \qquad (VII-68)$$

where

$$\sum_{K=1}^{4}XLEK(IG,E)=\text{total leakage from the reactor in group } IG$$

The sources in each group are given by;

$$SOSOR(IG)=\frac{\nu\cdot TOT}{\lambda}\sum_{IG=1}^{NG}\left[\chi(IG)\sum_{I=1}^{IREG}\Sigma_f(I,IG)\phi(I,IG)\right]+$$

$$\sum_{I=1}^{NREG}\sum_{\substack{K=1\\K\neq IG}}^{NG}\Sigma_R(I,K)\phi(I,K) \qquad (VII-69)$$

and the total source is determined as;

$$XE3=\sum_{IG=1}^{NG}SOSOR(IG) \qquad (VII-70)$$

CHAPTER VIII

FUEL DEPLETION ANALYSIS

[illegible] energy production proceeds in the reactor, the [illegible] occurs as a result of losses of fissile [illegible], build up and decay of fission [illegible] of the reactor materials due to neutron [illegible] of core composition changes in complex [illegible] the time and spatial variation in isotopic [illegible] depend on the neutron flux distribution which [illegible] position. Fortunately changes in core [illegible] relatively slowly (on time scales of hours [illegible] that the reactor core can be changed [illegible] by control element adjustments or [illegible] fission poison distribution. This makes [illegible] analysis of the rate equations describing [illegible] number densities is necessary, the [illegible] carried by performing a sequence of [illegible] calculations for each core composition [illegible] step of the burnup period.

[illegible] depletion analysis are considered [illegible] point of view of fuel management.

1. [illegible] reactivity loss rate associated with fissile [illegible] effects on the energy production during the [illegible]

2. The changes in power distribution caused by [illegible] by the effects of control poison [illegible] burnup.

3. Any change in fuel composition, with particular [illegible] losses of gaseous fission products [illegible] can be accurately evaluated.

The effects of depletion are evaluated by multiplying [illegible] reaction in the reactor into a node [illegible] depletion analysis in that zone [illegible] accounting separability in space and [illegible]

step in the evaluation is the calculation of a converged flux and/or power distribution for the spatial composition that existed at the beginning of the burnup step. This includes the amount of control material to yield a critical or near critical condition. The burn-up step length is chosen to be small enough so that the change in power distribution over the depletion interval is small. The power distribution is then extrapolated to the midpoint time step. Finally, the energy production rate is used to evaluate the changes in isotopic concentrations during a depletion step. The process is then repeated for subsequent time steps until the reactor is shutdown or the end of cycle with all control material removed, save that predicted for hot fully operations, startup and shutdown.

During the depletion process, the neutron spectrum within the energy groups will also be subject to change. This effect can be accounted for by recalculating the appropriate cross sections in each fuel type periodically during the depletion process or generating new fuel group constants for each fuel type at each step. This is equivalent to assuming equilibrium between the neutron spectrum and time over the depletion time step.

VIII-A THE BASIC EQUATIONS OF ISOTOPIC GENERATION AND DECAY

During the actual operation all the materials of which the reactor is composed are subject to change by neutron interaction. The general equation for isotope transmutation and radioactive decay is:

$$\frac{dN^j}{dt} = \cdots + \left[\lambda^j + \sum_{i=1}^{NG} \sigma_a^{i,j} \xi^{i,j} \phi^i(x)\right] + \lambda^{P3} N^{P3} + N^{P1} \sum_{i=1}^{NG} \sigma_c^{i,P1} \xi^{i,P1} \phi^i(x)$$

$$+ N^{P2} \sum_{i=1}^{NG} \sigma_c^{i,P2} \xi^{i,P2} \phi^i(x) + \sum_{i=1}^{NG} \gamma^{i,j-FP} N^j \sum_{i=1}^{NG} \sigma_f^{i,j} \xi^{i,j} \phi^i(x)$$

where

NG: number of groups

$\xi^{i,j}$: self-shielding factor of isotope j and group i

$\phi^i(x)$: energy flux over the considered region for group i

λ^j: decay constant of isotope j

$\sigma_a^{i,j}$: microscopic capture cross section of isotope j, in group i

M_1, M_2, M_3 : indices of the capture parents 1 and 2 and decay parent respectively

The time rate of change of the concentration of [illegible] in equation (VIII-1) is based on two loss modes and [illegible] gains. The two modes, by which the nuclei of [illegible] are lost, are:

1. The first term represents the loss by radioactive [illegible] of isotope j with decay constant λ^j.

2. The second term represents loss by neutron [illegible] with a spectrum averaged microscopic cross section [illegible] including fission and capture.

3. The third term in Equation VIII-1 represents [illegible] by radioactive decay of precursor, M^3, with [illegible] λ^{M_3}. Production of a given isotope [illegible] this one type of decay. As an example, M^{3} [illegible] by beta decay of I^{135}.

4. The fourth term represents production by [illegible] with a precursor species M^2 by neutron [illegible] with $\phi^{(2)}$. As an example, U^{235} is produced [illegible] on (n,γ) reaction in U^{234}.

5. The fifth term represents production by [illegible] by neutron capture with cross section $\sigma^{(1)}$.

6. The final term in Equation VIII-1 represents [illegible] loss for fission products, where the [illegible] product yield, γ^j, is dependent on [illegible] by isotope and the energy of the neutron [illegible].

[illegible] Equation (VIII-1) is nonlinear [illegible] cross sections are the [illegible] burn-up step length [illegible] spectrum, as [illegible] solution. Assuming a constant [illegible] Equation (VIII-1) [illegible] solution can be accomplished by [illegible] of other operating variables. One objective [illegible] the general equation is to eliminate [illegible] of the differential equations for [illegible] usually obtained at the expense of placing [illegible]

range of applicability.

All power reactors consist of both fissile and fertile materials. A fertile material is one that is capable of being transformed, either directly or indirectly, into a fissile material by neutron capture. Absorption of excess neutrons produced in the fission process by fertile material serves to extend the fuel cycle by creation of new fissile material. The two most important fertile nuclides are Th^{232} and U^{238}. The production chains for these isotopes are shown in Figure VIII-1 and VIII-2. Neutron capture in fertile nuclei exceeds the absorption in fissile

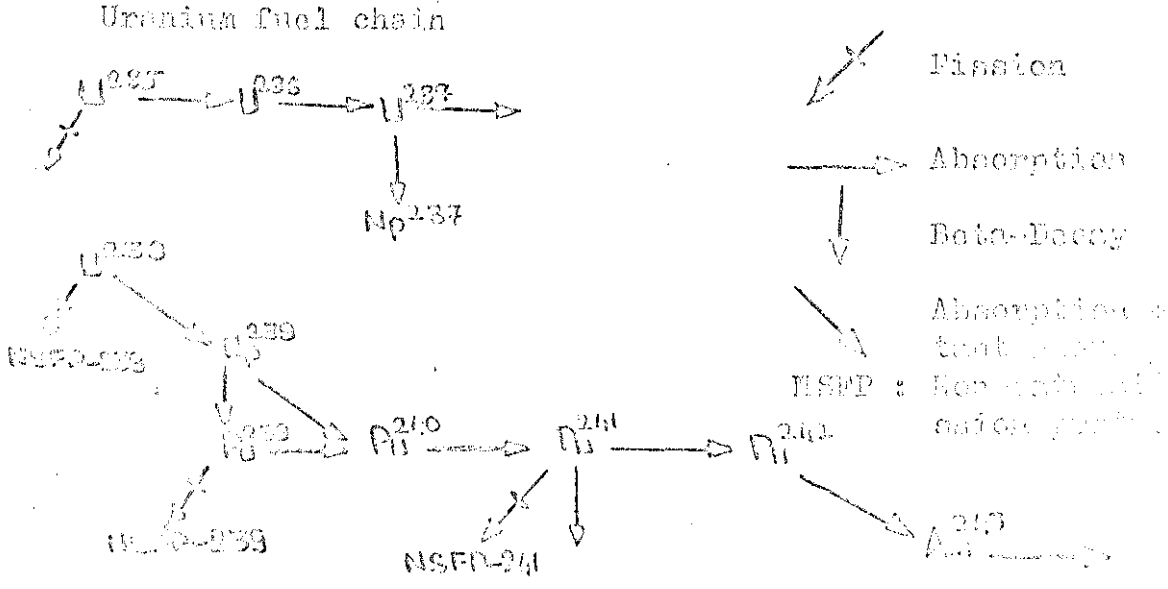


Figure VIII-1 Isotopic chains of interest in fuel depletion analysis.

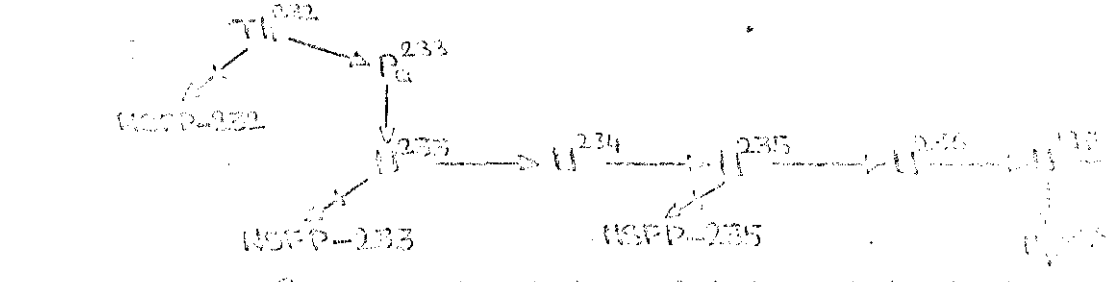


Figure VIII-2 Isotopic chains of interest in fuel depletion analysis.

terial, then the reactor is a net producer, or breeder of fissile material and is called a breeder reactor. The ratio of fissile material production to loss at any point in time is called the instantaneous breeding ratio. If the rate of fissile material production is less than the rate of loss of fissile material, the reactor is called converter reactor. Most thermal reactors are converters, although, breeding is possible in a thermal reactor that uses the Th^{232}-U^{233} system. The highest breeding ratios are possible with the U^{238}-Pu^{239} system in a fast neutron spectrum with which breeding ratios in the range of 1.25 to 1.4 are possible.

We first consider the transmutation chain for U^{238}, which is the most common fertile nucleus used in currently operating power reactors. In writing the equations for production and loss of the various isotopes in the chain we adopt the convention in which each isotope is described by a two digit superscript. The first digit in the superscript is the last digit of the mass number of the nucleus, and the second digit is the last digit of the mass number. The U^{238} concentration is thus again called N^{38} and Pu^{239} by N^{49}. The differential equations describing the chain in Figure VIII-1 are then:

$$\frac{dN^{38}}{dt} = -\sigma_a^{38} N^{38} \phi \qquad \text{(VIII-1)}$$

$$\frac{dN^{39}}{dt} = \sigma_c^{38} N^{38} \phi - \lambda^{39} N^{39} \qquad \text{(VIII-2)}$$

$$\frac{dN^{39}}{dt} = \lambda^{39} N^{39} - \lambda^{39} N^{39} \qquad \text{(VIII-3)}$$

$$\frac{dN^{49}}{dt} = \lambda^{49} N^{49} - \sigma_a^{49} N^{49} \phi \qquad \text{(VIII-4)}$$

$$\frac{dN^{40}}{dt} = \sigma_c^{49} N^{49} \phi - N^{40}(\sigma_a^{40}\phi) \qquad \text{(VIII-5)}$$

$$\frac{dN^{41}}{dt} = \sigma_c^{40} N^{40} \phi - N^{41}(\lambda^{41} + \sigma_a^{41}\phi) \qquad \text{(VIII-6)}$$

$$\frac{dN^{42}}{dt} = \sigma_c^{41} N^{41} \phi - \sigma_a^{42} N^{42} \phi \qquad \text{(VIII-7)}$$

In Equations (VIII-2) to (VIII-6), we have made several assumptions regarding the relative importance of production and loss terms. In Equation VIII-3 and 4, for instance, we have assumed for all anticipated flux values that the loss of U^{239} and Np^{239} by neutron absorption is negligible in comparison with loss by radioactive decay. We can obtain considerable additional flexibility if we assume that the time span of interest is long compared to the inverse decay constants of U^{239} and Np^{239}. Use of this assumption is that, for times long relative to these inverse decay constants, Pu^{239} is produced directly by neutron capture in U^{238}

$$\frac{dN^{49}}{dt} = \sigma_c^{28} N^{28} \phi - \sigma_a^{49} N^{49} \phi \qquad \text{(VIII-7)}$$

If we now redefine our independent variable to be the time integrated neutron flux or fluence

$$\Theta = \int_0^t \phi(t)\, dt \qquad \text{(VIII-8)}$$

we have the following coupled set of linear equations:

$$\frac{dN^{28}}{d\Theta} = -\sigma_a^{28} N^{28} \qquad \text{(VIII-9)}$$

$$\frac{dN^{49}}{d\Theta} = \sigma_c^{28} N^{28} - \sigma_a^{49} N^{49} \qquad \text{(VIII-10)}$$

$$\frac{dN^{40}}{d\Theta} = -\sigma_a^{40} N^{40} + \sigma_c^{49} N^{49} \qquad \text{(VIII-11)}$$

$$\frac{dN^{41}}{d\Theta} = \sigma_c^{40} N^{40} - \sigma_a^{41} N^{41} - \frac{\lambda^{41} N^{41}}{\phi} \qquad \text{(VIII-12)}$$

$$\frac{dN^{42}}{d\Theta} = \sigma_c^{41} N^{41} - \sigma_a^{42} N^{42} \qquad \text{(VIII-13)}$$

The last term in Equation VIII-12 is normally neglected in evaluating fuel composition changes. This introduces only a small error of less than 1% during reactor operation. The radioactive decay of Pu^{241} (half life 13.2 years) is important for the time periods between discharge from the reactor and reprocessing. For high burnup fuels, or fuels initially high

a mixture of fissile Plutonium isotopes, it is sometimes necessary to account for the neutron poisoning effects of other Plutonium isotopes such as Am^{241} and Am^{243}. Note that the loss term is always represented by the absorption cross section, σ_a, which includes capture and fission, while the production term is represented by the capture cross section of the previous isotope in the chain.

The solution of Equations VIII-11 to VIII-15 may be carried out in a straightforward fashion either numerically or analytically. Equations VIII-16, 21, 22, 23 give the analytical solution for isotopic build up equations for a series of four sequential isotopes. In this equations $N^1(0)$ is the initial concentration of the first isotope, σ_a^1 is the spectrum averaged microscopic cross section for absorption in isotope N^1 and σ_c^1 is the spectrum averaged microscopic cross section for capture to produce the next heavier isotope in the chain from isotope N^1. If none than one isotope of the chain is present at the beginning of a fuel burnup calculation the same series of equations can be used to determine the contribution of each initial isotope to the total concentration of the higher isotope. Note that the individual terms contain differences in cross sections and exponential terms, which may require that a large number of significant figures be carried in the calculation if the one group microscopic absorption cross sections are of the same order of magnitude in value.

Equation VIII-11 through 15 are easily solved by starting with the first and proceeding downward. The solution for N^1 is

$$N^1(\theta) = N^1(0)\, e^{-\sigma_a^1 \theta} \qquad \text{(VIII-16)}$$

Equation VIII-12 can be rearranged, this yields

$$\frac{dN^2}{d\theta} + \sigma_a^2 N^2 = \sigma_c^1 N^1 \qquad \text{(VIII-17)}$$

which is linear differential equation of the first order. If both sides are multiplied by the integration factor $e^{\sigma_a^2 \theta}$, the left side becomes a complete differential. Thus;

$$\left(\frac{dN^2}{d\theta} + \sigma_a^2 N^2 \right) e^{\sigma_a^2 \theta} = \sigma_c^1 N^1 e^{\sigma_a^2 \theta} \qquad \text{(VIII-18)}$$

so that;

$$d\left(N^2 e^{\Gamma_a^2 \theta}\right) = \Gamma_c^1 N^1 e^{\Gamma_a^2 \theta} d\theta \qquad \text{(VIII-19)}$$

If Equation VIII-16 is substituted into Equation (VIII-19) integration yields

$$N^2(\theta)\, e^{\Gamma_a^2 \theta} = \frac{\Gamma_c^1 N^1(0)}{\Gamma_a^2 - \Gamma_a^1} \cdot e^{(\Gamma_a^2 - \Gamma_a^1)\theta} + C \qquad \text{(VIII-20)}$$

where C is the integration constant. Integration over the limits $\theta=0$ to θ and $N(0)=0$ at $\theta=0$

$$N^2(\theta) = \Gamma_c^1 N^1(0) \left[\frac{e^{-\Gamma_a^1 \theta}}{\Gamma_a^2 - \Gamma_a^1} + \frac{e^{-\Gamma_a^2 \theta}}{\Gamma_a^1 - \Gamma_a^2} \right] \qquad \text{(VIII-21)}$$

The remaining equations can be solved by the same technique. The results of this solution can be obtained in the following forms;

$$N^3(\theta) = \Gamma_c^2 \Gamma_c^1 N^1(0) \left[\frac{e^{-\Gamma_a^1 \theta}}{(\Gamma_a^3 - \Gamma_a^1)(\Gamma_a^2 - \Gamma_a^1)} + \frac{e^{-\Gamma_a^2 \theta}}{(\Gamma_a^3 - \Gamma_a^2)(\Gamma_a^1 - \Gamma_a^2)} \right.$$

$$\left. + \frac{e^{-\Gamma_a^3 \theta}}{(\Gamma_a^2 - \Gamma_a^3)(\Gamma_a^1 - \Gamma_a^3)} \right] \qquad \text{(VIII-22)}$$

$$N^4(\theta) = \Gamma_c^3 \Gamma_c^2 \Gamma_c^1 N^1(0) \left[\frac{e^{-\Gamma_a^1 \theta}}{(\Gamma_a^4 - \Gamma_a^1)(\Gamma_a^3 - \Gamma_a^1)(\Gamma_a^2 - \Gamma_a^1)} + \frac{e^{-\Gamma_a^2 \theta}}{(\Gamma_a^4 - \Gamma_a^2)(\Gamma_a^3 - \Gamma_a^2)(\Gamma_a^1 - \Gamma_a^2)} \right.$$

$$\left. + \frac{e^{-\Gamma_a^3 \theta}}{(\Gamma_a^4 - \Gamma_a^3)(\Gamma_a^2 - \Gamma_a^3)(\Gamma_a^1 - \Gamma_a^3)} + \frac{e^{-\Gamma_a^4 \theta}}{(\Gamma_a^3 - \Gamma_a^4)(\Gamma_a^2 - \Gamma_a^4)(\Gamma_a^1 - \Gamma_a^4)} \right] \qquad \text{(VIII-23)}$$

VIII-B FISSION PRODUCT POISONING

Several hundred fission product isotopes are present in partially depleted fuel as a result of direct yield from fission, radioactive decay of fission products, neutron capture in a fission product, or a combination of the latter two processes. The fission product inventory of the reactor core is one of problems that must be considered by the fuel management engineer in studying the behavior of each fuel cycle.

Hence, in order to estimate the reactivity effects due to fission product poisoning, one must calculate the concentration of the poisoning isotope N(t) as a function of time. To calculate N(t), one must solve the rate equations describing the various production and decay processes that can affect the concentration which will be illustrated with an example for the build up of Xe^{135}.

Xe^{135} is the most significant fission product poison because of its large neutron absorption cross section and relatively large fission yield. Actually Xe^{135} can be formed not only directly as a fission product but also through the β^--decay of Te^{135}. A portion of the production-decay scheme for the A=135 chain is shown in Figure VIII-3

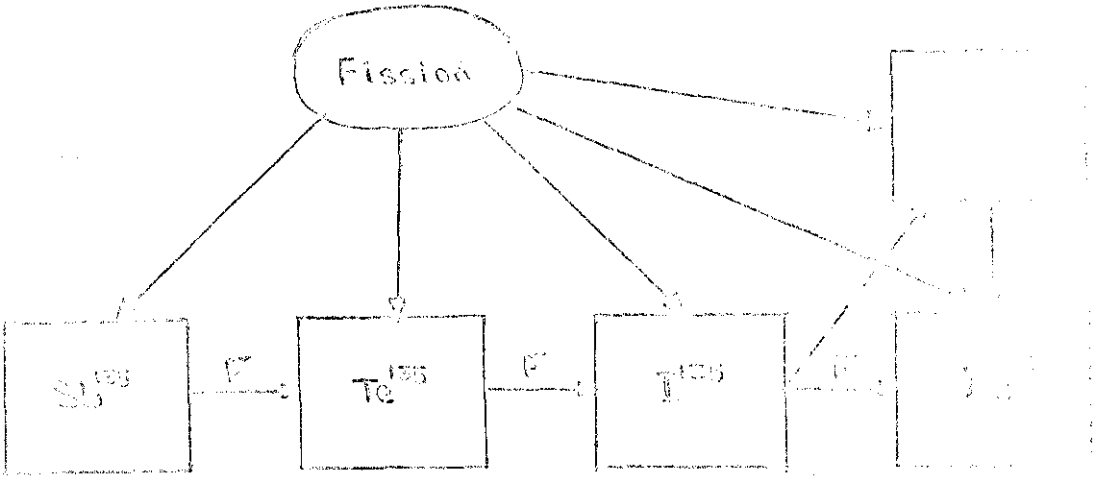


Figure VIII-3 A portion of the decay scheme for A=135.

Unfortunately this rather complicated decay scheme can be considerably simplified by assuming that the decay of I^{135} is instantaneous. Furthermore we will also ignore the short isomeric state Xe^{135} and assume that all I^{135} nuclei will decay directly to the ground state of Xe^{135}. Hence the effective decay scheme to be studied is shown in Figure VIII-4.

Let us denote the atomic number densities of the two nuclides as $N^I(t)$ and $N^X(t)$ respectively. Furthermore let γ_I and γ_X be the effective fraction of the fission products which are I^{135} and Xe^{135} while λ_I and λ_X are the β decay constants for these two isotopes. Using these parameters, one can then write the following equations describing the simplified decay scheme illustrated in Figure VIII-4

Iodine

$$\frac{\partial N^I}{\partial t} = \gamma_I \Sigma_f \phi - \lambda_I N^I \qquad \text{(VIII-2.)}$$

Xenon

$$\frac{\partial N^X}{\partial t} = \gamma_X \Sigma_f \phi + \lambda_I N^I - \lambda_X N^X - N^X \sigma_a^X \phi \qquad \text{(VIII-3.)}$$

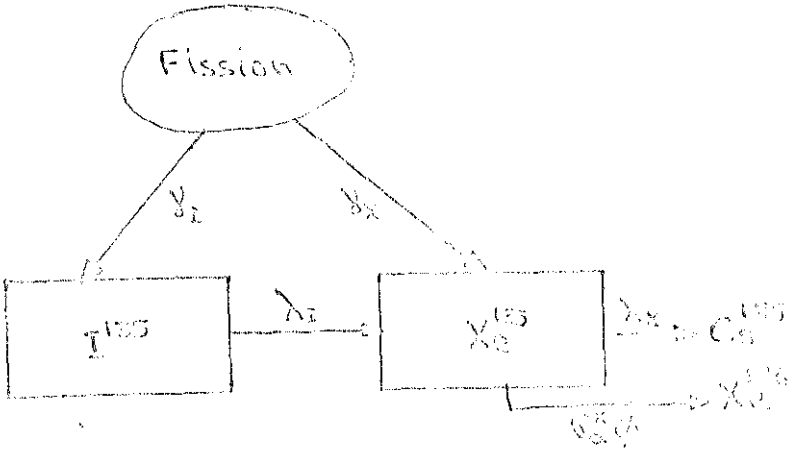


Figure VIII-4 A simplified decay scheme for I^{135}

Notice that a loss term has been included in the Xenon balance equation to account for the fact that neutrons are lost to deplete the Xe^{135} concentration. Before proceeding to solve equation VIII-25 one needs to solve Equation VIII-24 the solution of which is;

$$N^I(t) = \frac{\gamma_I \Sigma_f \phi}{\lambda_I} \left(1 - e^{-\lambda_I t}\right) \qquad \text{(VIII-}\ldots\text{)}$$

substituting this solution into Equation VIII-25 and solving to determine the Xe^{135} concentration as a function of time

$$N^X(t) = \frac{(\gamma_I + \gamma_X)\Sigma_f \phi}{\lambda_X + \sigma_a^X \phi} \left[1 - e^{-(\lambda_X + \sigma_a^X \phi)t}\right] + \qquad \text{(VIII-}\ldots\text{)}$$

$$\frac{\gamma_I \Sigma_f \phi}{\lambda_X - \lambda_I + \sigma_a^X \phi} \left[e^{-(\lambda_X + \sigma_a^X \phi)t} - e^{-\lambda_I t}\right]$$

That is, the concentration of these fission products in a reactor operating at constant flux will eventually reach an equilibrium value for which the production of the fission is just balanced by the decay and burnup of the poisons. These equilibrium concentrations may also have been determined directly from the rate equations VIII-24 and 25 themselves by merely setting $dN/dt = 0$.

VIII-C SUBROUTINES DEPL, SUBD, DBURN, SUBB, BBB and SUBDET

At any time step, these subroutines calculate the absorption factors, perform the flux normalization and solve the depletion equation.

Subroutine DEPL is used to calculate the macroscopic cross sections and the normalized flux. For the calculation of the β_{eff} number it is necessary to have both the fast and the group constants. Self shielding factors are

the subprogram SHIED. The method of calculating the self shielding factors is the same as that described in the subprogram SHUCH. Also the same procedure, explained in NCHM, is followed to calculate the normalization factor and the normalized flux as.

After calculating the normalized flux, it must be saved for a multi time step starts. For this reason, the loss and sources terms of the depletion equation are calculated again.

There are two loss terms, explained before. Absorption is denoted by VABS(j) ;

$$VABS(j) = \sum_{IG=1}^{NG} \sigma_a(IG,j)\, \xi_j(IG,j)\, \phi(L,IG) \qquad (VIII.28)$$

the radioactive decay is denoted by DEC(j);

$$DEC(j) = \lambda(j) \qquad (VIII.29)$$

There are four source terms which are also an application of fore. Fission is denoted by;

$$VFIS(j) = \sum_{IG=1}^{NG} \sigma_f(IG,j)\, \xi_j(IG,j)\, \phi(L,IG) \qquad (VIII.30)$$

Capture cross section is defined as absorption cross section minus the fission cross section and thus the gain due to capture is;

$$VCAP(j) = VABS(j) - VFIS(j) \qquad (VIII.31)$$

Gain due to beta decay;

$$BETA(j) = DEC(j) \qquad (VIII.32)$$

Fission yield is;

$$YIELD(J,I) = GAM(J,I,N1) \qquad \text{(VIII-35)}$$

Decay constants and fission yields have been given as input.

After that, subprogram DEPL calls subprogram DETM for constituting the depletion matrix which is called DEPM. It is a triangular matrix. Diagonal elements of DEPM is combination of

$$WABS(J) + DEC(J)$$

The other elements of the depletion matrix are placed in a [illegible] subprogram SPLIT which splits the given depletion matrix MAT into NFICHN independent of fuel and [illegible] fission product chains. Each chain is characterized by [illegible] vectors NSPLIT(L) which is the index of the first nuclide of chain L,

NUCA(L), (L=1,2 ... NCHAIN) is the width of the [illegible] matrix. After splitting the depletion matrix, subprogram [illegible] and DECEP solve each depletion-submatrix equation [illegible] by using an analytical approach.

CHAPTER IX

DISCUSSION AND SUGGESTIONS FOR FURTHER WORK

This study was to form the second part of a larger [illegible] concerning the possibility of power production [illegible] U^{233} generation from Th^{232} in a conventional PWR [illegible] adapted for the AKKUYU plant. The first part has [illegible] PWR oriented code GETLS developed by K. Tonadow, [illegible] Subject of the engineering GfKS (Gesellschaft für Kernverfahrenstechnik Schiffbau und Schiffahrt mbH.) to generate [illegible] constants for reactor cells made up of varying [illegible] fuel elements in which the Uranium component is [illegible] percent levels between 12 and 20% U^{235} by weight. [illegible] tions for supercells containing lumped control [illegible] rated by that study (21)

In this work the intention was to study the [illegible] tion depletion program "THERMOS" in two dimensions [illegible] of approach so as to prepare an enlarged [illegible] ment and adapt the code to the UNIVAC-1106 system [illegible] University. This has been accomplished to a [illegible] extent. Several trial runs proved to be not possible due to [illegible] errors encountered in attempts to have access to the [illegible] THERMOS that was supposed to be generated by the [illegible] THROD. The possibility of using the card input [illegible] has not been precluded because of the large [illegible] data required by THERMOS. Thus the study [illegible] a detailed outline of the code and debugging of [illegible] program by adaptation to UNIVAC-1106, when.

Further work along these lines could involve [illegible] removing the obstacle to successful utilization of [illegible] by THERMOS and then using the code to analyze [illegible] reactors composed of different cell regions for which [illegible] may not be generated by GETLS. There is also [illegible] approach to the design of a PWR that would [illegible] of breeding without sacrificing the other desirable [illegible] of the PWR, such as UO_2 placing a Thorium rich shell [illegible] of the core would result in high conversion but [illegible] would be adversely affected at least for a few [illegible]

until the contribution from U^{233} that is building up reaches a significant level. Also such Thorium rich cells near the core center would require highly enriched Uranium cells in other regions to assure sufficient k_{∞} values and thus sufficient core lifetime. On the other hand, an inclination to place the Thorium rich cell more at the periphery of the core would be bad for neutron economy since Thorium conversion is more efficiently done with low energy neutrons and also because the neutrons in peripheral regions would be lost through leakage from the core anyway. Thus the core designer would have to try different configurations while being guided by considerations of this and choose the design that performs best according to the criteria of Thorium conversion, power production, uniformity of peak, Xenon concentration, amount of excess reactivity available initially and throughout the core lifetime and finally the core lifetime itself incorporating the fuel cycle economics.

APPENDIX A

INPUT DATA PREPARATION

The maximum number of bytes available to the program on the IBM-360 is not yet definitely settled, and is likely to undergo changes in the near future. Therefore, in view of possible restrictions on the machine available, the maximum dimensions of ERMINUS can not be specified on this manual, but can be indicated parametrically. The numerical values of the maximum, for the present version of ERMINUS now operating, are given in appendix B, so that future changes of the program restrictions will only imply the [illegible] of appendix B.

The correspondence between the logical peripheral units used by ERMINUS and the physical units of the IBM-360 (tapes, disks or drums), is not definitely established, being susceptible of changes, due to either possible modification of the program or to future new computer configurations. The correspondence between physical and logical units obtained in the present version of ERMINUS is given in appendix C.

The input data have been divided into 25 cards each (which may contain one or more cards):

1 : TITLE CARD (18A4)

Col. 1-56	Title of the problem.
Col. 57-72	Leave these columns blank (they are used in RESTART problems).

2.: CARD No. 2 (24I3)

Col. 1-3	NG (≤KGD)	=	number of groups.
Col. 4-6	NREG (≤IREG)	=	number of regions.
Col. 7-9	NCMP (≤NCD)	=	number of compositions.
Col. 10-12	NIS (≤NIS)	=	maximum isotopic index.
Col. 13-15	NPY (≤JYD)	=	number of rows.
Col. 16-18	NPX (≤JXD)	=	number of columns. N.B.: It must be NPX=1, as, for a spatially [illegible] (JPX=1). NPX/2, even (for [illegible]).
Col. 19-21	NT	=	maximum number of outer boundaries.

Col. 22-24 IFDIT = 0 the point fluxes are not printed.
= 1 the point fluxes are printed only for specified groups.
= 2 the point fluxes are printed for all groups.
(the point power is printed in any [illegible]

Col. 25-27 IFG = 1 the initial flux approximation, for the time step zero, is read from tape.
= 0 is read from cards, per prcnp
=-1 is read from cards, per co[illegible] per group.
=-2 is read from cards, per region and group.

Col. 28-30 ILAM = 1 the initial eigenvalue approximation for the time step zero, is read from tape.
= 0 is read from cards, or is calculated by the program.

Col. 31-33 ISIG = 1 the first guess of the dominance ratio for the time step zero, is read from tape.
= 0 is read from cards or calculated by the program.

Col. 34-36 IOM = 1 the spectral radii of the fundamental matrices, in the first call by iteration of the time step zero are read from tape.
= 0 are calculated by the program.
=-1 are read from cards.

Col. 37-39 IMACR = If this field is zero or left blank the macroscopic cross sections are not read

Col. 40-42 IMACR1= If this field is zero or left blank shielding factors are not read

Col. 43-45 IPRINT= print index. If IPRINT = [illegible] program prints the solution at [illegible]

3.: CARD No. 3 (24I3)

Col. 1-3 NGRINT = last time step
The time steps are numbered start from zero.

Col. 4-6 NRUN = last time step to be completed in present run (NRUN<[illegible]
If NRUN=NGRINT, the program ends [illegible]

the diffusion calculations of the ... me-step IGRINT.
If IRUN<IGRINT, the program ... ter the computation of the ... sities and the saving of ... start, and before the first ... and the diffusion calculations of the time step IRUN+1.

Col. 7-9 NGEOM = 0 x, y geometry.
= 1 r, z geometry.

Col. 10-12 IDIAG = 1 the reactor is symmetric about ... 45° main diagonal. In this case it must be:
NPX=NPY and NPX*(NPX+1)/2≤NPD.
= 0 no diagonal symmetry.

Col. 13-15 ICOND = 0 the boundary conditions are the ... for all groups.
= 1 the boundary conditions are group dependent.

Col. 16-18 IPOW = 0 only one power all through the ... time.
= 1 the power is specified for each ... step.
= 2 the power is specified for each ... time-step.
If IGRINT=0, it must be IPOW=0.

Col. 19-21 IBK = 0 one buckling.
= 1 buckling per group.
= 2 buckling per group and per ...
= 3 buckling per group and ...

Col. 22-24 ISYST = 0 the microscopic cross ... ven in burns, and the ... in Bell and ( ) Bell ...
= 1 the cross section ... the number densities ...

Col. 25-27 NSHZ = 0 the self shielding factors ... ated by formula (IV-1)
= 1 the self shielding factors ... ated by the polynomial ...

Col. 28-30 ICRIST = 0 straight burnup.
= 1 search of the dilution factor 0.
= 2 regionwise prescribed ... trol isotope number density.
= 3 boundary search.

Col. 31-33 NCRIT = maximum number of criticality it[illegible]
hote that, in the boundary [illegible]
criticality iteration [illegible]
displacement of one"elementary step" [illegible]
one mesh row).

Col. 34-36 NUCL = number of time-dependent isotopes. [illegible]
time-dependent (or burnable) isotopes
numbered from 1 to NUCL (NUCL[illegible]

Col. 37-39 NIF = number of fuel isotopes. All [illegible]
from 1 to NIF are considered [illegible]
It must be NIF≤NUCL. (NIF≤[illegible]

Col. 40-42 NIP = number of fission product [illegible]
isotopes numbered from (NIF+1) [illegible]
ARE CONSIDERED FISSION PRODUCTS.
It must be (NIF+NIP)≤NUCL.

If the field 34-36(NUCL) is zero or left blank, the [illegible]
automatically assumes the standard isotopic chain of [illegible]
It must be NUCL≤NIS

4 : SPECIFICATION FOR THE GROUP-FLUX PRINTING

This set of one or more cards (24I3), present only [illegible]
is equal to one, on card no.2, specifies the [illegible]
$F_1, 2, \ldots, NG$

Col. 1-3 IP(1) = 1 the point flux of group 1 is [illegible]
= 0 is not printed

Col. 4-6 IP(2) = the same meaning for the [illegible]
so on for all groups. [illegible]
or more cards are needed.

5 : CARD No.5 (7E10.5)

Col. 1-10 AUTCRI = eigenvalue λ_c to be [illegible]
criticality search. [illegible]
= minimum allowed eigenvalue [illegible]
NISE= 0. If the multiplic[illegible]
at some time step, [illegible]
λ_{min}, the calculation is [illegible]
field contains zero or [illegible]
the program assumes AUTCRI [illegible]

Col. 11-20 AUT = initial eigenvalue [illegible]
If this field is zero or [illegible]
ram assumes AUT = 1. [illegible]
used only if IMAT = 0 [illegible]

Col. 21-30 SIGMA = initial guess of the [illegible]
(= ratio between the [illegible]
eigenvalue λ, if the eigenvalue [illegible]

dered by decreasing modulus). It must be $\zeta < 1$. If this field is left or contain zero, and ISCH=0 on card no.2, ζ is calculated by the program.

Col. 31-40 ETA = convergence criterion for the eigenvalue searches (ICRIT = 0). This search is interrupted when $|\lambda - \lambda_c| < \text{ETA}$

Col. 41-50 EPS = pointwise convergence criterion :

$$\frac{\lambda_{max} - \lambda_{min}}{2\lambda} < \text{EPS}$$

Generally EPS = 10^{-3} is an adequate

Col. 51-60 POWER = reactor power (watt), if only one for all through the lifetime is (IPOW = 0 on card no.3). If IPOW leave this field blank.
If the reactor is symmetric about two axes, 1/2 or 1/4, respectively, the reactor total power must be This holds also if the power time-step or small time-step

Col. 61-63 DEL = Convergence criterion for If this field is zero or left program sets automatically DEL=

Col. 64-66 TAU = Convergence criterion for factor. If this field is zero or the program sets automatically TAU=

6 : CARD No.6 SPECTRAL RADII OF GAUSS-SEIDEL This sub consists of one or more cards (FORMAT 8F10.5) if
Col. 1-10 GGA(1) = spectral radius of Gauss-Seidel for group 1
Col. 11-20 GGA(2) = same for group 2.
And so forth, up to GGA(NG).

7 : BOUNDARY CONDITIONS
In ... tions on each external side of the reactor, of type :

$$\alpha^i \phi^i + \beta^i D^i \frac{\partial \phi^i}{\partial n} = 0 \qquad (i = 1, 2, \ldots\ldots)$$

where $\alpha^i \geq 0$, $\beta^i \geq 0$, $\alpha^i + \beta^i > 0$.
This sub consists of one card (8E9.4) if ICOND = 0 or if ICOND = 1 .

Col. 1-9 α_1^i
Col. 10-18 β_1^i } for the top side (row 1)

Col. 19-27 α_2^i
Col. 28-36 β_2^i } for the left side (column 1)

Col. 37-45 α_3^i
Col. 46-54 β_3^i } for the bottom side (row NPY)

Col. 55-63 α_4^i
Col. 64-72 β_4^i } for the right side (column NPX)

8 : SHUFFLING TIME-STEPS

This set of one or more cards (24I3), present only if [illegible] is greater than zero, is to specify the vector KSU(K), [illegible] numbered, starting from one to NGRINT.
If KSU(K) = 1, the program performs the shuffling; [illegible] diffusion calculation of the time-step K. If KSU(K) = [illegible] shuffling is performed. It is not possible to perform [illegible] shuffling at time-step zero.

9 : SMALL TIME-STEP DIVISION

This set of one or more cards (24I3), present only [illegible] is greater than zero, specifies the subdivision of each time-step into small time-steps.
The first card contains:
Col. 1-3 NSA(1) = number of small time-steps, into which time-step 1 is divided.
Col. 4-6 NSA(2) = number of small time-steps, into which time-step 2 is divided.
And so forth, up to NSA(NGRINT).

It must be $\sum_{K=1}^{NGRINT} NSA(K)$ = total number of small time-steps less than or equal to maximum number of small time-steps

10: TIME-STEP LENGTHS

This set, present only if NGRINT = 0 , contains one or more cards (F10.5) :
Col. 1-10 DELTAT(1) = length (hours) of the time step 1
Col. 11-20 DELTAT(2) = same, for time step 2
And so forth, up to DELTAT(NGRINT), using as many cards as necessary.

11 : TIME-STEP POWERS
This set, present only if NGRINT > 0 and IPOW = 1, contains one or more cards (7E10.5). The first card is :

Col. 1-10 W(1) = power (watt) for the time step 1
Col. 11- 20 W(2) = power (watt) for the time step 2
and so forth, up to W(NGRINT).
At any time step K, the fluxes are normalized in such a way that :

$$\frac{1}{\lambda} \sum_{i=1}^{NG} \int_{Reactor} \nu^i \Sigma_f^i(r)\, dV = W(K)$$

12 : SMALL TIME-STEP POWERS

This set, present only if NGRINT > 0 and IPOW=2, is made of NGRINT sets of cards (7E10.5), one for each time step.
The set I contains the powers of all small time-steps into which the time-step I is divided.
Initialize a new card when changing time-step.
The above card sets are read by the subprogram PINPAC. The card sets below are read by the subprograms CINDAC and PINPAC

13 : Δx-MESH SPECIFICATION (along the X axis)
Each card is divided into 6 parts [6(E9.3,I3)] of 12 columns each. Each part is constituted by a 9 column field (E9.3) and a 3 column field (I3), and specifies a couple (Δx, C) where Δx is a mesh space length (in cm) and C is the cell up to which this value is extended. All the C must be given in an increasing order, and the last one must be IMX.

14 : Δy-MESH SPECIFICATION (along the Y axis)
The same rule as before are holding. The last specified value of C must be coincident with IMY.
N.B.- This set of cards must be omitted in diagonal symmetry problems (IDIAG=1).

15 : SPECIFICATION OF THE INITIAL COMPOSITIONS
One or more cards (24I3)
Col. 1-3 IMIX(1) = initial composition of region 1
Col. 4-6 IMIX(2) = initial composition of region 2

The compositions are numbered according to the order in which the corresponding number densities are specified (Cf. setno.22 : NUMBER DENSITIES PER COMPOSITION)

16 : SPECIFICATION OF THE REGIONS AND CONTROL AREAS
The geometric specification of the regions is made through the so called "OVERLAY" method employed in many diffusion programs (e.g. refs. 1 and 2) for the composition specification. The lay-out of the regions is inputed by the sequential specification of rectangular blocks of a given region index. The specification of the rectangular blocks is made by inputing sets of 6 integers :

Col. 1-3 i_r = region index of the block

Col. 4-6 c_1 = left column bounding the block ($1 \leq c_1 \leq NRX$)

Col. 7-9 c_2 = right column bounding the block ($1 \leq c_1 \leq c_2 \leq NPZ$)

Col. 10-12 r_1 = upper row bounding the block ($1 \leq r_1 \leq NPY$)

Col. 13-15 r_2 = lower row bounding the block ($1 \leq r_1 \leq r_2 \leq NPY$)

Col. 16-18 = Generally these columns are to be left blank. Only when ICRIT=3 this field is used to indicate the region index of the "follower". (The follower is defined as the region which replace the region i_r when the moving boundary is withdrawn).

The specification is continued in columns 19-36, 37-54, and 55-72 using as many cards as necessary.

17 : BLANK CARD
A blank card indicates the end of the region overlay and control area specification.

18 : SPECIFICATION OF THE ISOTOPIC CHAINS
This set of cards is present only if NUCI>0 (Card no.3). there must be NUCI cards (2A4, 3I4, 2E10.5), one for each time dependent isotope, folowing order of the isotope index from one to NUCI.

Col. 1-8 Isotope name (any alphanumeric characters). It is suggested that the name start with column 1.

Col. 9-12 Nc_1 = index of the first capture parent

Col. 13-16 Nc_2 = index of the second capture parent

Col. 17-20 N_β = index of the decay parent

Col. 21-30 λ = decay constant

Col. 31-40 atomic weight (gram/mole)
We recall that the indices No_1, No_2, No_p must be less than the index of the considered isotope.

19 : INITIAL FLUX GUESS
This set of one or more cards (7E10.5) must be omitted if IFG=1.
If IFG=0, NG values must be supplied.
If IFG=-1, there are NG sets, one for each group, on which the initial flux guesses for all compositions from 1 to NCMP are specified.
If IFG=-2, there are NG sets, of one or more cards (one set per group), each containing NBMG values.

20 : BUCKLINGS
This set of one or more cards (7E10.5) is for the specification of bucklings.
If IBK = 0 (Card no.3, columns 19-21) only one card (7E10.5 is present, containing the B^2.
If IBK = 1 there must be one or more cards containing NG bucklings, one for each group.
If IBK = 2 there must be NG sets , one for each group, on which the bucklings for all compositions from 1 to NCMP are specified.
If IBK = 3 there must be NG sets, of one or more cards (one set per group), each containing NBMG bucklings.

21 : INFORMATION CARD
There must be one card (2I3) containing :
Col. 1-3 NEC = number of isotopes whose number densities are given per composition (0≤NEC≤NTC).
Col. 4-6 NEMIR = number of isotopes whose number densities are given per region (0≤NEMIR≤NTC-NEC).
Col. 7-9 NEC = number of compositions to be obtained by derivation (0≤NEC≤NCM).
Col. 10-12 IPUN = 1, the number densities of the first NBMG isotopes are punched on cards (7E10.5) at each time step, before the bucklings.
IPUN = 0, no punch cards.
These punched cards can be used to input the number densities per region in other problems.

22 : NUMBER DENSITIES PER COMPOSITION
This set of cards, present only if NEC ≠ 0, is constituted of :

22.a) one or more cards (24I3) containing the isotope indices of the NEC isotopes whose number densities are given in(22.b)

22.b) for each isotope declared in (22.a), one or more cards (7E10.5) containing NCH' number densities, one per composition.
Initialize a new card when changing isotope.

23 : NUMBER DENSITIES PER REGION
This set of cards, present only if NEMIR $\neq 0$, is arranged in the same way as the set "Number densities per composition" Read REGION instead of "COMPOSITION".

24 : LOGARITHMIC DERIVATIVES
This set of cards, present only if NEC $\neq 0$ is constituted of :

24.a) One or more cards (24I3) containing the indices of the NEC compositions which have logarithmic derivatives.

24.b) NEC sets of cards (7E10.5), one for each composition, containing the logarithmic derivative C_j , $i=1,2,\ldots,IG$.
Initialize a new card, when changing the composition.
If $C_j>0$, the composition under consideration is a "partial material" with respect to the group i; in this case the function φ^i is not evaluated in the mesh points inside the composition, but it must satisfy, on the boundary points, the condition is

$$D^i \frac{\partial \varphi^i}{\partial n} = - C^i \varphi^i$$

If $C_j=0$, the composition under consideration is a normal diffusion material with respect to the group i.

25 : χ^i SPECIFICATION
This set is made up of one or more cards (7E10.5) containing the fission spectrum integrals χ^i $(i=1,2,\ldots,IG)$ for all groups.
It must be $\chi^i \geq 0$ and $\sum_{i=1}^{IG} \chi^i > 0$.

STOP
DATA

26 : DATA FOR THE UNIFORM SEARCH
Only if ICRISE = 1, there must be one card (7E10.5) containing :
Col. 1-10 DIMIN = Θ_{min} = minimum permissible value of the dilution factor .
Col. 11-20 DIMAX = Θ_{max} = maximum permissible value of the dilution factor .

27 : CONTROL LIST FOR THE REGIONWISE PROGRAMMED SEARCH
This set, present only when ICRITE = 2 , specifies the control list. It is made of as many cards (18I3, 2X,4) as the number of control banks. The first 18 fields, of three columns each, contain the indices of the regions belonging to the same bank.
Each bank can be constituted by one or more regions, but obviously not more than 18.
The last two fields, of 9 columns each, contain :
Col. 55-63 N_{min} = minimum permissible value of the control isotope number density, for the bank under consideration
Col. 64-72 N_{max} = maximum permissible value of the control isotope number density ($N_{min} \leq N_{max}$).
These number densities are given in Bailard or in nuclei/cm^3 according to the option INNT in card no.3 .
The same region can be repeated in two or more different banks. The maximum number of control bank is NBTSF, and the total number of all region indices appearing in this set must not be greater than NTRL.
The control isotope (of index NUCL+1) retains the given values of its number densities, specified per composition or per region, in the regions which do not appear in the control list. These values are, on the contrary, ignored for the regions belonging to the control list.

28 : BLANK CARD (only if ICRITE = 2)
A blank card indicates the end of the control list specification.

29 : CONTROL LIST FOR THE BOUNDARY SEARCH
This card set, present only if ICRITE=3, specifies the control list in the boundary searches. It is made up of as many cards(24I3) as the number of control banks. The first 22 fields, of 3 columns each, are devoted to the specification of the rectangular control areas which belong to the considered bank. Each bank can be constituted by one or more areas with the only obvious limitation of 22. The following two data are then specified :

Col. 67-69 y_{min} = row number which represents the upper limit of the moving boundary for the bank under consideration.
Col. 70-72 y_{max} = row number representing the lower limit of the moving boundary ($y_{min} \leq y_{max}$)

The same control area can be repeated in two or more different banks. The maximum number of control banks is NBLK. The entries of the control list (i.e. all the area indices appearing in the cards above) must not be more than NAT. Recall that the control areas are numbered in the same order that they are specified in SPECIFICATION OF THE REGIONS AND CONTROL AREAS.

30 : BLANK CARD (only if ICRISE=3)
A blank card indicates the end of the control list specification in the boundary searches.

31 : LIBRARY AND SELF SHIELDING PARAMETERS
It is possible, in EXCEL, to specify many sets of microscopic cross section libraries, called library sets and many sets of self-shielding coefficients, called self-shielding sets.
It is necessary, then, to assign to each initial composition a well determined LIBRARY SET and a SELF-SHIELDING SET.
The following card (24I3) provides general information :

Col. 1-3 NBL=INX1= total number of library sets (NBL≤NBT)
If NBL>0 , NBL sets of microscopic cross sections must be supplied consecutively, by means of as many data sets in EXCEL file "SPECIFICATION OF THE LIBRARY SETS"
If NBL = 0, possible only if a PARK RESTART case is dealt with, the program takes library data from the RESTART TAPE .

Col. 4-6 NBS=INX2= total number of self-shielding sets (NBS≤NBT)
If NBS>0 , NBS sets of self-shielding coefficients must be supplied successively by means of as many card sets 33: SPECIFICATION OF ONE SELF-SHIELDING SET, ending with the card 34: SELF-SHIELDING SET ASSIGNMENT which assigns the various self-shielding sets to the compositions.
If NBS=0, no self-shielding data (neither SELF-SHIELDING SPECIFICATION nor SELF-SHIELDING ASSIGNMENT) are supplied on cards but the program reads it from the RESTART TAPE if the case under

consideration is a restart case, otherwise sets all the self-shielding factors equal to one for all groups and isotopes, if it is not a restart case.

Col. 7-9 NGP = number of coefficients $a_{\ell+1}$ (NGT $\geq$ 7)

SPECIFICATION OF ONE LIBRARY SET

The description of this data set applies to one generic library set. If library set number (NLS) is greater than one, NLS such sets of data must be supplied consecutively by the GELS code. Each set will take a distinctive number called library set number, according to the order in which such sets appear in the NGELS file.

For each isotope, whose microscopic data are to be supplied there must be the following sets of data in the NGELS file.

a.) Name of the isotope. This name is used only for output purposes for the nonburnable isotopes.

b.) Index of the isotope. If this index is greater than NIS, library data of this isotope are ignored.

c.) IDEP = 0, This isotope is included in the summation (over TER-IV Formula(IV-15)), and its self-shielding factors are functions of the argument (IV-15).

= 1, this isotope is not included in the summation (IV-15), and its self-shielding factors are functions of the argument (IV-15).

= 2, this isotope is included in the summation (IV-15) and its self-shielding factors are functions of the argument (IV-16)(that is of its number density only).

= 3, this isotope is not included in the summation (IV-15), and its self-shielding factors are functions of the argument (IV-16).

This field is read only in the first library set, if many are present, then its data are extended also to the other sets.

d.) If this alphanumeric field is not blank (e.g. contains the word SCATTER), a complete scattering matrix must be supplied for this isotope.

If this field is blank, no such matrix is supplied, but it is assumed that the removal occurs only from one group to the next lower one (single down-scattering)

e.) This field generally must be left blank. The word SET END must be punched in the next isotope of the set.

f.) The microscopic transport cross sections σ_{tr}^{i} (i=1,2,...NG).

g.) The microscopic absorption cross sections σ_{a}^{i} (i=1,2,...NG).

h.) The microscopic removal cross sections σ_{R}^{i} (i=1,2,....NG) to the next group.

If the isotope is a fuel isotope, that is its index is less than or equal to NFT , data i.), k.), l.), m.) must be supplied, otherwise they are omitted.

i.) The microscopic fission cross sections σ_{f}^{i} (i=1,2,....NG)

k.) The microscopic fission cross sections times the number of neutrons per fission $\nu\sigma_{f}^{i}$ (i=1,2,...NG)

l.) The energies per fission e^{i} (i=1,2,...NG) (joule/fission)

m.) The fission yields $\sigma_{fR}^{j\rightarrow}$ (j= NIP+1, NIP+2,....,NIP+NIP) of the isotope under consideration (I) for all fission products

n.) This set is present only if the stage d.) has the word 'SCATTER. It is made of NG sets containing the microscopic removal cross sections $\sigma_{R}^{i\rightarrow j}$ (j=1,2,...NG)

32 : LIBRARY ASSIGNMENT
The first card (24I3) contains :
Col. 1-3 the library set number assigned to composition 1
Col. 4-6 the library set number assigned to composition 2 and so forth, up to the last composition NCMP. If NCMP > 24, the assignement is continued on one or more cards.
The library set numbers are the progressive numbers in which the library sets are given.

33 : SPECIFICATION OF ONE SET -SHIELDING SET
The description of this set of cards applies to one generic self-shielding set. If more than one self-shielding set are present (NSS > 1) NSS such sets of cards must be supplied consequtively. Each set will take a distinctive number, or index (called set number) according to the order in which such set appears in the input deck.
For each set, more blocks of self-shielding coefficients can be given. One block is made of NG·NIP coefficients (for all groups).

33.a) The first card (24I3) contains :
Col. 1-3 NBT(I) = total number of blocks of self-shielding

coefficients of the set K under consideration. It must be NBT(K) ≠ 0 .

Col. 4-6 block number assigned to the isotope no. 1.
Col. 7-9 block number assigned to the isotope no. 2.
and so forth for all the NIS isotopes.
If NIS > 24 , the assignment is continued on one or more successive cards, starting with the field 1-3.
The block numbered "zero" is a block having the first coefficient of all groups equal to one, and all the other coefficients equal to zero. This block is implicitly defined by the program, and causes all the self-shielding factors to be 1 .

33.b) The blocks of coefficients are specified consequtively. Each block must have NG cards (7E10.5), one for each group in increasing order, with the self-shielding coefficients from 1 to NGT.
Remember that the number densities in formula (IV-16) are in Szilard even if they have been inputted as nuclei/cm^3
There is limitation to the total number of self-shielding coefficients; it must be :

$$NG \cdot NGP \sum_{I=1}^{NIS} NBT(K) \leq NCOF$$

34 : SELF-SHIELDING ASSIGNMENT
The first card (24I3) contains :
Col. 1-3 self-shielding set assigned to the composition no.1.
Col. 4-6 self-shielding set assigned to the composition no.2 .
and so forth. If NCMP > 24 the assignment is continued on one or more cards.

Recall that the numeration of the self-shielding sets is based on the order in which the cards SPECIFICATION OF SELF SHIELDING SETS appear in the input.
The self-shielding set no. 0 is automatically defined by the program as giving all the self-shielding factors equal to 1, so its assignment to a given composition is equivalent to setting equal to 1 all the self-shielding factors of the composition.

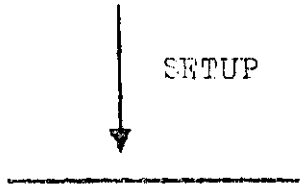
LIBRA

35 : FUEL SHUFFLING LIST
This set of cards must be supplied for any time-step K such

that NFU(K)=1, to be performed in the present run (Cfr. SHUFFLING TIME-STEP)
The first card (24I3) contains :
Col. 1-3 NLSM = number of elements of the following list L(I), I=1,2,....,NLSM.
Col. 4-6 L(1) = first element of the list.
Col. 7-9 L(2) = second element of the list.
and so forth. If NLSM > 24 the list is continued on one or more cards. The meaning of L(K) is :

L(K) = 0 the region K remains unchanged.
= M the number densities of the burnable isotopes in the region K are replaced by the ones of the region M.
= N the number densities of the burnable isotopes in the region K are replaced by the ones of the composition N.

If NLSM = 0, there must be only one card, filled with zeros or blanks.
If NLSM > 0, it is obvious that the vector L(K) must be supplied for the regions from 1 to NLSM. The regions successive to NLSM do not undergo any shuffling.



APPENDIX B

PROGRAM RESTRICTIONS

The present version of WREBUS has the following maximum dimensions:

Maximum number of library sets	KBL = 5
" " " self shielding sets	KBS = 5
" " " compositions	KCD = 40
" " " self shielding coefficients	KCOF = 5000
" " " groups	KGD = 15
" " " fuel isotopes	KIF = 20
" " " fission products	KIP = 20
" " " isotopes	KIS = 40
" " " burnable isotopes	KIV = 29
" " " control banks	KLIST = 100
" " " mesh points	KPD = 10000
" " " regions	KREG = 300
" " " time-steps	KRINT = 50
" " " control areas	KROD = 100
" " " small time-steps	KSMAT = 150
" " " elements in the control list	KTRL = 400
" " " rows	KYD = 200
" " " columns	KXD = 200

APPENDIX C

PERIPHERAL UNIT CONFIGURATION

Logical unit	Physical unit	Function
2	tape or disk	to store the finite difference coefficients and the data for the STRONG RESTART
3	tape or disk	
4	disk	banal
9	tape or disk	to store the fluxes
11	tape or disk	
10	tape or disk	to store the data for the WEAK RESTART

When required, the aforementioned tapes should be mounted on the physical units available to programmers. For instance on the IBM-360/65 at ISPRA, the available physical units are as follows:

2-389 , 2-38A , 2-38D (9 tracks)

2-38C , 2-38E , 2-38F (7 tracks)

(the double number such as 2-389 specifies the same physical unit but accessible from two different channels.)

Moreover a tape is needed for off-line punching of number densities, if required. The procedure for card punching is subjected to the rules holding in the Computer Center.

The correspondence between logical and physical units is left to the programmer's choice and is defined by the DD cards (with other informations concerning the use of peripheral units).

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