A STUDY OF THE TWO DIMENSIONAL MULTIGROUP DIFFUSION ANALYSIS CODE: EREBUS

by

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APPROVAL OF READERS

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ÖZET

Bu çalışmanın amacı EREBUS isimli, çok gruplu difüzyon [illegible] iki boyutlu geometride çözerek kritiklik [illegible] yapan bilgisayar programını detaylıyla incelemektir. EREBUS [illegible] ENEL ve CISE'nin yardımıyla M. Console, A. D[illegible] ve F. [illegible] geliştirilmiş olup Boğaziçi Üniversitesindeki [illegible] 1105 sistemine uygulanmıştır. Programın dili FORTRAN IV'[illegible].

Bu bilgisayar programı difüzyon denklemini iki boyutlu [illegible] veya r-Θ) geometride sonlu farklar yöntemiyle [illegible] ederek çözmekte ve gerekli olan mikroskopik tesir kesitleri [illegible] bilgisayar programları tarafından hazırlanmaktadır. [illegible] GKSS'nin (Gesellschaft für Kernenergieverwertung in Schiffbau und Schiffahrt mbH.) yardımıyla K. P[illegible], F. [illegible] G. Schulz tarafından geliştirilmiş olan GRTS kodu [illegible].

EREBUS bir ana program ve muhtelif alt programlardan [illegible] yazılmıştır. İşlev aşağıdaki şekilde sıralanabilir:

1. Giriş bilgilerinin okunması, kontrol edilmesi, [illegible] edilmesi ve yazılması.

2. Grup sabitlerinin ve makroskopik tesir kesitlerinin [illegible] lanması.

3. Difüzyon denkleminin sonlu farklar yöntemiyle [illegible] edilmesi ve katsayıların hesaplanması.

4. Sonlu fark denklemlerinin çözümü.

5. Yakıt elemanlarındaki yanma miktarlarının ve [illegible] belirlenen zaman dilimlerinde hesaplanması.

6. Elde edilen bilgilerin düzenlenerek yazılması.

ABSTRACT

The purpose of this study is to examine and expl[illegible] computer code EREBUS. It is a multi-group diffusion depletion code in two dimensions, with criticality searches. This [illegible] has been developed by M. Consolo, A. Daneri, and [illegible] under the auspices of EURATOM-FIAT-ARS and is adapted to the [illegible] 370 system at BOĞAZİÇİ UNIVERSITY. Program [illegible] FORTRAN IV.

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

The microscopic cross section data for this code [illegible] generated by various codes but, GRLS, developed by K. [illegible] and G. Schulz under the auspices of GKSS (Gesellschaft für Kernenergieverwertung in Schiffbau und Schiffahrt) [illegible] designed specifically for this purpose.

EREBUS consists of one main program and several subroutines, the major sections of which perform the following functions:

1. Processing of the input data, including checking [illegible] data.

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

3. Calculation of the coefficients for the finite difference equations used to approximate the group diffusion equations together with the interface and boundary conditions.

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

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

6. Editing of the selective information for [illegible] and plotting.

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NOMENCLATURE

SYMBOL CHARACTERIZE

[illegible](J) : Absorption term for the J^{th} isotope

[illegible] : Actual power density

A(J) : Atomic weight of the J^{th} isotope

Av : Avogadro Number

J : Burnable (time dependent) isotope index

M : Composition index

[illegible] : Decay constant

[illegible] : Dilution factor

[illegible] : Effective volume of the reactor

[illegible] : Fission source term

YIELD : Fission yield

[illegible] : Form factor

[illegible] : Integrated actual power

[illegible] : Integrated actual source

PF : Integrated actual volume flux

[illegible] : Losses due to absorption, removal and [illegible]
leakage

[illegible] : Macroscopic absorption cross section

[illegible] : Macroscopic cross section for energy [illegible]

[illegible] : Macroscopic fission cross section

[illegible] : Macroscopic removal cross section

N(L) : Number density in region L

[illegible] : Neutron flux

L : Region index

SCSOR : Scattering collision source

: Self-Shielding factor

$W(J)$: Total weight of the J^{th} burnable isotope in [illegible]

$W(M,J)$: Weight of the J^{th} burnable isotope in one [illegible]

$W(I,J)$: Weight of the J^{th} burnable isotope in region I

CHAPTER I

INTRODUCTION

The purpose of this study is to examine and explain the computer program REXDUS which is a multigroup diffusion code in two dimensions, with criticality searches. This code is designed for effective use in the computers of the IBM-360 series and [illegible] which have large directly addressable storage. It is developed by M. Gonnelli, A. Benassi and E. Salina under the auspices of [illegible] in Fortran IV language and has been adapted to [illegible] system at Boğaziçi University.

[illegible] is designed to solve problems involving the finite difference representation of diffusion theory treating [illegible] group equations with arbitrary intergroup scattering. [illegible] problems may be solved by using an analytical formulation [illegible] analysis.

A nuclear reactor is a device in which nuclear [illegible] are so arranged that a self sustained [illegible] reaction can occur in a controlled manner. The required condition for a stable, self sustained chain reaction in a nuclear reactor is that exactly one of the neutrons produced in a fission subsequently succeeds in inducing another fission. In other words, one fission must lead to another, and if this [illegible] the neutron population within the system will remain [illegible]. If, on the other hand, each fission eventually leads to [illegible] fission, the fission rate will [illegible] and so will the neutron population [illegible]. Conversely, a transient of the sort for which the [illegible] dies out can result from an insufficient [illegible] of fissions induced by a single fission of the [illegible].

These ideas can be expressed conveniently in terms of the multiplication factor. This is defined as the ratio of the number of fissions in any one generation to the number of fissions in the immediately preceding generation. When this [illegible] is exactly equal to unity the number of fissions in each [illegible] population is a constant rate and such a system is [illegible] critical. If the multiplication factor is greater than unity, the number of fissions increases with each succeeding generation, in which case, 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 [illegible] in a multiplying medium can be written as;

$$\nabla\cdot D(r,E)\nabla\phi(r,E,t) - \Sigma_t(r,E)\phi(r,E,t) + \chi(E)\nu\Sigma_f(r,E)\phi(r,E,t) = \frac{1}{v(E)}\frac{\partial}{\partial t}\phi(r,E,t) \quad (I-1)$$

When the system is in a steady state, the time derivative [illegible] equation would simply vanish and the resulting equation [illegible] be describing a critical system. In search for criticality [illegible] one can modify the above equation by the introduction [illegible] by λ as follows;

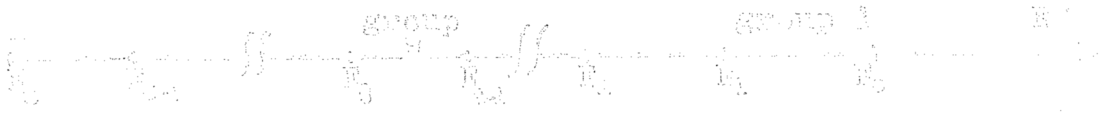
$$-\nabla\cdot D(r,E)\nabla\phi(r,E) + \Sigma_t(r,E)\phi(r,E) = \frac{\chi(E)}{\lambda}\nu\Sigma_f(r,E)\phi(r,E) \quad (I-2)$$

In passing from Equation (I-1) to equation (I-2) the source term has been multiplied by 1/λ and the time derivative has been [illegible] Physically this mathematical step corresponds to [illegible] of the real system source by a factor 1/λ so as to [illegible] obtains time independent i.e. critical system described by Equation (I-2). However, if the solution of the latter [illegible] [illegible] then the system described by both equations [illegible] only the actual system under investigation [illegible] at steady state. However if λ turns out to be [illegible] would have reduced the source in the actual [illegible] to obtain a time independent or critical situation [illegible] clearly mean that the actual case is supercritical [illegible] a solution of Equation (I-2) giving [illegible] [illegible] of the actual system [illegible] [illegible] steady state [illegible] [illegible] expected solution of Equation (I-2) [illegible] system parameters, such as [illegible] which case the actual system described by Equation [illegible] [illegible] with the time independent system described by Equation (I-2). In other words, we have arrived at [illegible] that can sustain a time independent [illegible] symbol. As will be made clear later in this work this factor [illegible] is exactly the same thing as the multiplication factor [illegible] ed above.

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 the multigroup problem can be solved by the source iteration [illegible]. 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 equations in the two dimensional case. In stage four, the solution of the resulting equations will be discussed.

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

We will now allow the neutron flux to depend on energy. Rather than treat the neutron energy variable E as a continuous variable, we will immediately discretize it into [illegible] intervals or groups as schematically shown below:



Notice that [illegible], we are using a backward indexing scheme, [illegible] physically to the fact that the neutron usually loses energy during its lifetime and mathematically to the fact that one usually solves the discretized equations starting with the highest energies and working successively to lower energies.

It would be possible to discretize $\phi(r,E)$ by [illegible] only to be defined at each energy mesh point E_g. However, it is more convenient to define the discretized fluxes as [illegible] integrals of $\phi(r,E)$ over the energy range of each group. Then the multigroup fluxes $\phi_g(r)$ represents the total flux of neutrons with energies E, in the group $E_g < E < E_{g-1}$. When we come to determine equations governing the behaviour of $\phi_g(r)$, 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 experience changes in energy by, for example, being scattered from one group to another. Also, fission neutrons will usually be born 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 description. The ability to describe a reactor adequately with a relatively small number of energy groups is not simply fortuitous, but rather is a consequence of a careful choice of the energy-averaged group constants that characterize the neutrons in each group. Hence the calculation of such group averaged cross sections or multigroup constants 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. We will then rederive these equations in a more rigorous fashion which is also more amenable to a numerical solution. Finally we will discuss the common calculational strategies used to solve this set of coupled partial differential equations.

Perhaps, the most straightforward manner in which one can arrive at the form of the multigroup diffusion equations is to apply the concept of the neutron balance to a given energy group by tabulating the ways in which neutrons can enter or leave this group. Consider then a typical energy group g.

After a bit of reflection, it should be apparent that a neutron balance would read at steady state as follows:

$$\begin{bmatrix}\text{Change}\\ \text{Per Unit}\\ \text{Time}\end{bmatrix} = -\begin{bmatrix}\text{Absorbed}\\ \text{in}\\ \text{group g}\end{bmatrix} + \begin{bmatrix}\text{Source neut-}\\ \text{rons appearing}\\ \text{in group g}\end{bmatrix} - \begin{bmatrix}\text{neutrons scat-}\\ \text{tering out of}\\ \text{group g}\end{bmatrix} + \begin{bmatrix}\text{[illegible]}\\ \text{[illegible]}\\ \text{[illegible]}\end{bmatrix}$$

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 either remove it from group i, or if it is initially in another group j, scatter it into energy group i. We will [illegible] the probability for scattering a neutron from group j to the group i, as $\Sigma^{j\to i}$. Then,

$$\Sigma_R^i = \sum_{\substack{j=1\\ j\neq i}}^{NG} \Sigma^{i\to j} \qquad \text{[illegible]}$$

is the cross section for removal from group i.

We will similarly define an absorption cross section characterizing the group i, Σ_a^i, and a source term $S^i(x)$ giving the rate at which source neutrons appear within this group. Finally we will define a diffusion coefficient D^i so that the leakage from group i can be written within the diffusion approximation as $-\nabla D^i \nabla \phi^i$. If we combine all of these terms, we find a mathematical representation of the time independent balance relation. The diffusion equations solved by EREBUS are thus:

$$-\nabla\cdot D^i(x)\nabla\phi^i(x) + \left[\Sigma_a^i(x) + \Sigma_R^i(x) + (D^i B^2)\right]\phi^i(x) = \text{[illegible]}$$

$$\sum_{j=1}^{i-1} \Sigma^{j\to i}(x)\phi^j(x) \qquad \text{[illegible]}$$

$$S^i(x) = \chi^i \sum_{j=1}^{NG} \nu\Sigma_f^j(x)\phi^j(x) \qquad \text{(fission source term)} \quad \text{[illegible]}$$

$$T^i(x) = \sum_{\substack{j=1\\ j\neq i}}^{NG} \Sigma^{j\to i}(x)\phi^j(x) \qquad \text{(removal source term)} \quad \text{[illegible]}$$

x represents the spatial variables, either x,y or r,z; i is the group index, NG is the total number of groups. The physical interpretation 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

$\Sigma_r^{i\to j}$: the macroscopic removal cross section from group i to [illegible]

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 EREBUS perform the following functions:

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

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

3. Calculation of the coefficients for the finite difference equations used to approximate the group diffusion equations together with interface and boundary conditions.

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

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

6. Editing of selective information for printing and plotting.

In order to have EREBUS readily modifiable for adaptation to other machines of the IBM-360 series, but with different size available storage, the dimensions of the program (the maximum number of groups, compositions, regions, mesh points, fissile isotopes and so on) are parametric.

The numerical values of these parameters, for the present version of EREBUS, are given in appendix B.

A brief account of the physical model employed is given. At the beginning of core life, the elements comprising [illegible] generally are uniformly distributed, but as burnup proceeds [illegible] spatially, composition becomes nonuniform. Hence, it is [illegible] to take into account the spatial variation of the group constants, namely, the diffusion coefficient D, the fission cross section and the neutron production rate per unit of flux $\nu\Sigma_f$.

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 nuclear densities are assumed uniformly distributed within the same region.

CHAPTER II

EREBUS consists of one main program and thirty-three subprograms. The schematic diagram of EREBUS is given in Figure II-1. The main program calls the subprograms OVER-1, OVER-2, ..., OVER-[illegible]. It controls the number of time steps. If time step number (KC[illegible] is greater than the last time step number (KGRINT) 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 adjustable. 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:

KBL:	Maximum	number	of	library sets
KSS:	"	"	"	self shielding sets
KCD:	"	"	"	compositions
KGD:	"	"	"	groups
KUF:	"	"	"	fuel isotopes
KIP:	"	"	"	fission products
KIS:	"	"	"	isotopes
KIV:	"	"	"	burnable isotopes
KRINT:	"	"	"	time steps
KROD:	"	"	"	control areas
KLIST:	"	"	"	control banks
KREG:	"	"	"	regions
KSMAT:	"	"	"	small time steps
KSEL:	"	"	"	elements in the control [illegible]
KXD:	"	"	"	X meshes
KYD:	"	"	"	Y meshes
KSOP:	"	"	"	self shielding coefficients

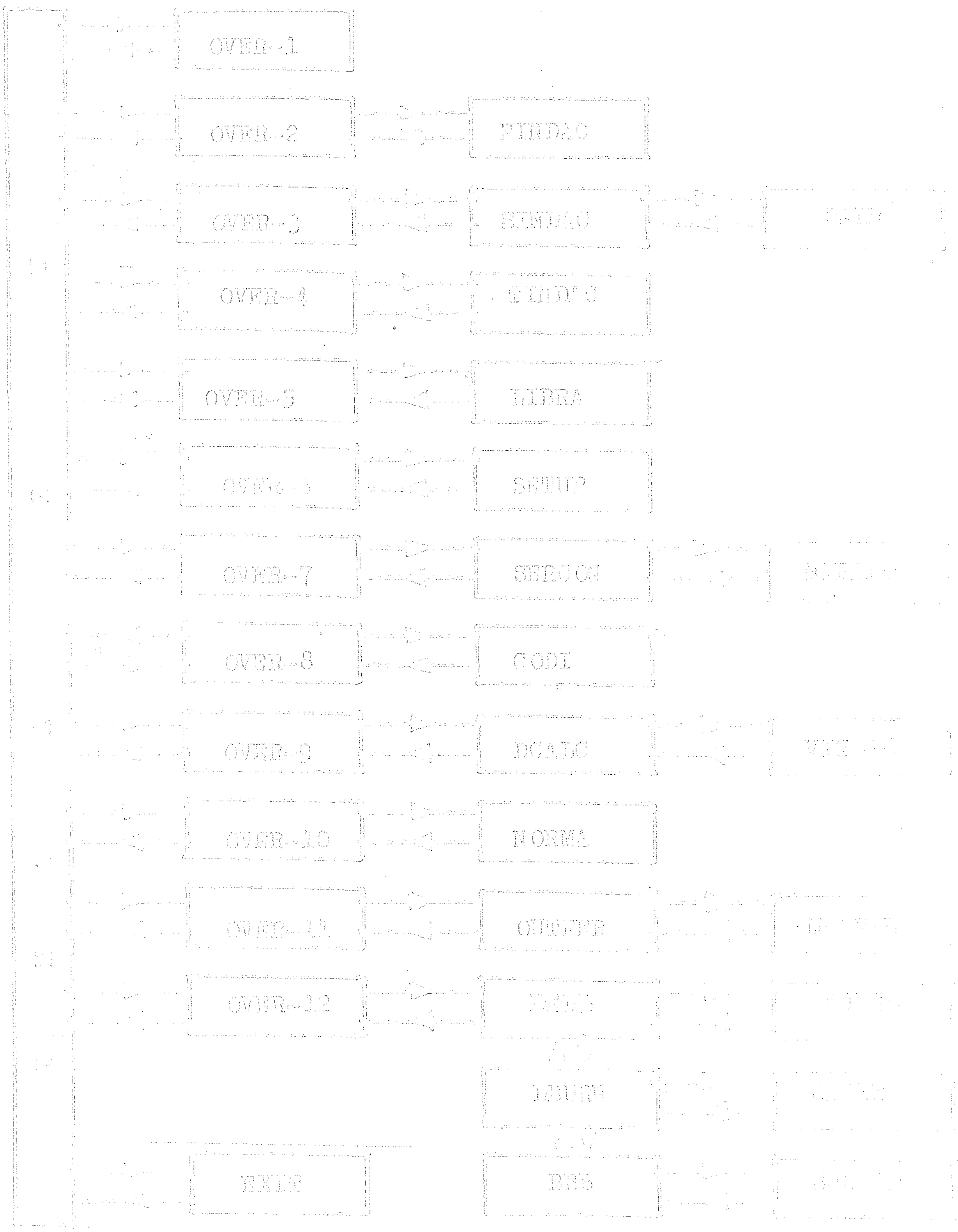


Figure IV-1 The schematic diagram of REMSUS

KPD: Maximum number of mesh points
IPR: " " " print indices
NOT: " " " arrays taken in common

The following conditions have to be observed:

$KIP \geq KIF$ $\quad$ $KIS \leq KCD$
$KIV \leq 60$ $\quad$ $KLIST \geq 5$
$KXD \quad KYD$ $\quad$ $KROD \geq 5$
$KCD \leq KREG$ $\quad$ $KTRL \geq 5$

$KPD \geq NPX.NPY$ or $(KXD \cdot KYD)$
$KPD \geq (NPX + 1) \cdot NPX/2$ or $(KXD + 1) \cdot KXD/2$ for diagonal symmetric problems.

$$KCOF \geq NG \cdot NGP \sum_{K=1}^{NSS} NBT(K)$$

where

NGP: Number of the coefficients
NBT(K): Number of blocks of self shielding coefficients of the set K

The values of the above parameters are printed as output by [illegible]. Length of the common region is calculated and if it is [illegible] checked, otherwise a return is made to the main. Variable [illegible] counts the possible errors and if INXIT > 0, then again [illegible] [illegible].

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. Next, the data is controlled for any possible errors and existence of any leads to an abortion.

EREBUS is an "overlay program" constituted by main and subprograms which are illustrated in Figure II-1. Subprograms OVER-2, OVER-3, ..., OVER-12 are used only to call related subprograms. Subprograms FINDAC, SINDAC, DELR, TINDAC and LECTR read, check, reorder and print out the input data. The input data have been divided into 35 card sets. One set may contain one or more cards. Input data set is given in APPENDIX A.

There are three types of starts in EREBUS 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 in a criticality search, can be restarted from the last (or the last but one) criticality iteration being performed at the time of interruption.

Moreover, if the restart is made using also the flux tape prepared by the program, the STRONG RESTART is practically equivalent to restart of a problem from the every point where it was interrupted, except for a loss of time negligible with respect to the total computational time.

c. Work restart: By this type of restart, a problem can be restarted just after the number density evaluation, relative to the last executed time step, or to any other preceding time step.

III-A FINDAC

FINDAC is the subprogram referenced by OVER-2.

The geometric specification of the reactor is given in 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 axes, 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. These are shown in Figure III-1.

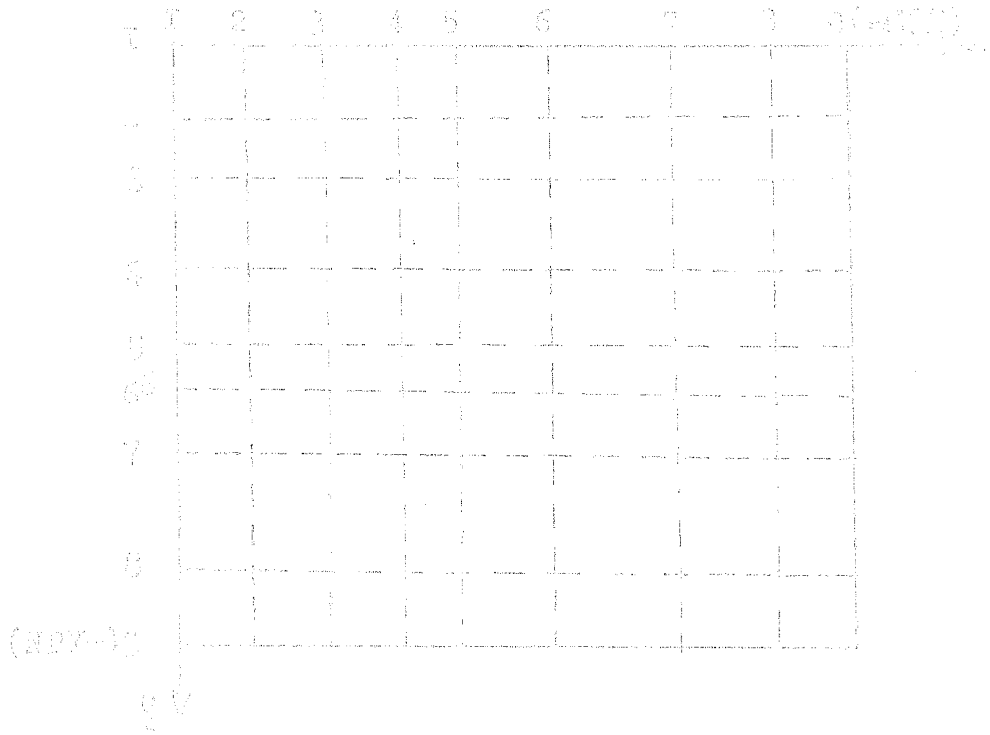


Figure III-1 Sample reactor core mesh layout

The reactor is divided into regions in each of which the program performs an average burn-up, that is, assigns the same average isotopic number densities and hence the same macroscopic cross sections to all rectangular meshes belonging to a given region. A region can also be made up of disjoint sets of rectangular meshes.

Two or more regions can have the same initial composition. In the following and also in the program print-outs, 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 separate composition.

III-A-4 BOUNDARY CONDITIONS

The boundary conditions are given as

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

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 $(-\frac{\nabla\phi}{\phi}) \neq 0$ when $\alpha^i \neq 0$ and $\beta^i \neq 0$.

If $\alpha^i = 0.5$ and $\beta^i = 1$ condition (III-1) represents a vanishing inward but non-zero outward current in diffusion theory.

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

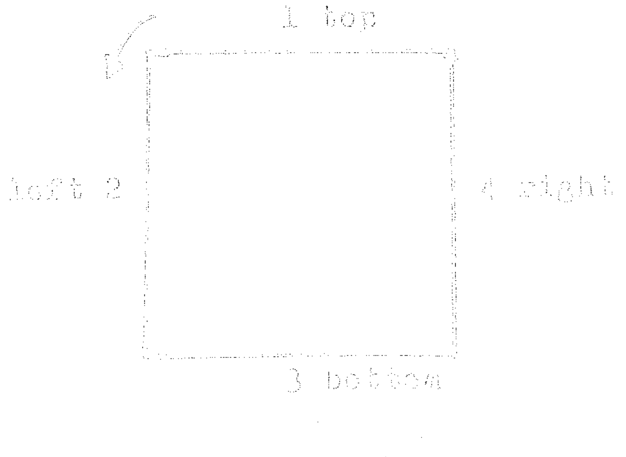


Figure III-2

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

If $\alpha^i=\beta^i=0$, 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 $\alpha^i=0$ and [illegible] (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 remaining condition (vanishing inward current), it sets the indicator as α^i/β^i. This fraction must always be greater than zero.

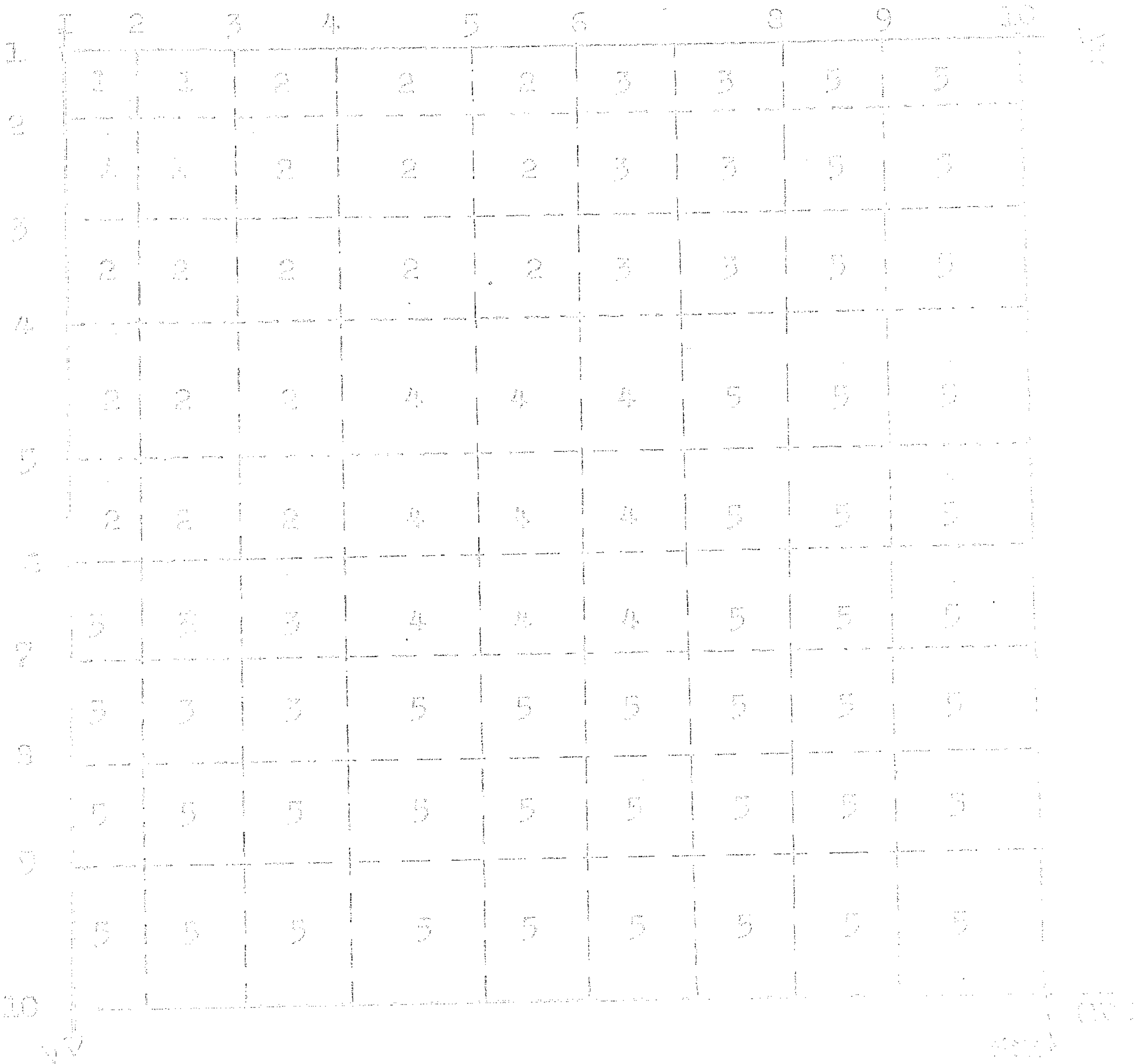
III. 8 SUBROUTINE SINDAC AND DELR

These subprograms read, check, reorder and print out some of the input data. The geometric specification of the reactor has been given as input data in the subprogram FINDAC. The distances between rows and columns are called mesh space lengths, and are given as input in cm.

The geometric specification of the regions is made through the so called "overlay" method employed in many diffusion codes (e.g. ref.1 and 2) for the composition specification. The lay-out of the regions is inputted by a sequential specification of rectangular blocks of a given region index. Any of such blocks can cover totally or partially the preceding ones.

Referring to Figure III-3, the regions [illegible] problem is described as follows:

Suppose the reactor were divided into 5 regions. In each of them the program performs an average meaning, that is, it assigns the same average isotopic number densities and hence the same macroscopic cross sections to all rectangular meshes belonging to a given region. Vertical (columns) and horizontal (rows)



1	1	2	2	2	3	3	5	5
1	1	2	2	2	3	3	5	5
2	2	2	2	2	3	3	5	5
2	2	2	4	4	4	5	5	5
2	2	2	4	4	4	5	5	5
3	3	3	4	4	4	5	5	5
3	3	3	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5
5	5	5	5	5	5	5	5	5

Figure III-3 Example reactor core region system.

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

REGION OVERLAY

Region number	Colomn number	Row number
5	1 - 10	1 - 10
4	4 - 7	4 - 7
3	1 - 4	1 - 4
2	1 - 6	1 - 6
1	1 - 3	1 - 3

Subprogram SINDAC calculates the region and composition volumes. Mesh space length between rows is Δy and columns Δx, the other dimension is unity. Then the volume of one mesh square is

$$VOL = \Delta x . \Delta y \qquad \text{(III-[illegible])}$$

A region consists of one or more mesh squares. The volume of one region is found by summing over the mesh grid volumes which belong to the same region. The same way is used to calculate the other region volumes. VOL(L) is the volume of region L.

After the region volumes, composition volumes are calculated by the program by summing up to the region volumes having the same composition so as to obtain the composition volumes. VOL(M) is the volume of composition M.

III-B-4 NUCLIDE CHAIN SPECIFICATION

Fuel depletion analysis is concerned with predicting the long-term changes in reactor fuel composition caused by exposure to neutron flux during reactor operation. Such changes have an important bearing on the operating life of a reactor, as well as on the stability and control.

A variety of nuclear processes must be monitored during a depletion study. These include, of course, the depletion of fissile nuclides (fuel burn-up). However one must also account for the conversion of fertile isotopes into fissile isotopes and the production of numerous fission products. Finally, one should monitor the reactivity balance to ensure continued criticality usually by determining the change in reactivity over a period of core operation and then adjusting control poison to compensate for this reactivity change.

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, Pm^{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 monitored depend on the particular fuel used in the core. The isotopes of interest in both Uranium and Uranium-Thorium fueled reactors are indicated in tables 1 and 2 respectively.

TABLE-1

No	Name	1st capture parent	2nd capture parent	Decay parent	Fissionable	Fission product
1	U-235	--	--	--	Yes	No
2	U-236	1	--	--	Yes	No
3	U-238	--	--	--	Yes	No
4	Pu-239	3	--	--	Yes	No
5	Pu-240	4	--	--	Yes	No
6	Pu-241	5	--	--	Yes	No
7	Pm-149	--	--	--	No	Yes
8	Sm-149	--	--	7	No	Yes
9	I-135	--	--	--	No	Yes
10	Xe-135	--	--	9	No	Yes
11	Lumped fission product	--	--	--	No	Yes
12	Boron	--	--	--	No	Yes
13	Burnable poison	--	--	--	No	[illegible]

TABLE-2

No	Name	1st capture parent	2nd capture parent	Decay parent	Fissionable	Fission product
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 3.

The number densities of the first NUCL+1 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 the first (the control isotope) can be specified only per composition.

In the criticality searches by means of a control isotope variation (ICRISE = 1,2 on card no.3 columns 28-30), the program assumes, as control isotope, the isotope no NUCL+1.

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 weak restart problems. In the latter case, the number densities and the logarithmic derivatives are the ones read from the restart tape.

III.C SUBROUTINE TINDAC

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.

KREBUS 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.

TINDAC 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 NAT1=9, and printed out.

[illegible] introduce λ, the multiplication factor [illegible] stable fission chain reaction and thereby [illegible] fraction rate of fission energy, [illegible] in such a way that the rates of [illegible] are balanced by the rate of fission [illegible] We can express this requirement in [illegible] the neutrons play the central role [illegible] this reaction let us focus our [illegible] A given neutron will be "born" [illegible] scatter about the reactor [illegible] "death" in either an absorption [illegible] the reactor. Certain numbers of these [illegible] fissile or fissionable nuclei and [illegible] thereby leading to the birth of new fission [illegible] new "generation" of neutrons. Suppose [illegible] measure the number of neutrons in [illegible] then define the ratio of [illegible] factor λ characterizing the [illegible]

[illegible] factor = Number of [illegible] / Number of [illegible] generation.

[illegible] since the number of fission neutrons [illegible] proportional to the number of fission events [illegible] (recall that each fission reaction [illegible] fission neutrons), we could have [illegible] the number of fission events in [illegible] is a bit awkward, however, since [illegible] to determine the neutron generation [illegible] neutrons may induce fission [illegible] fission reaction. Others may [illegible] before inducing fission. Some [illegible] fissions at all, but will [illegible] or leak out of the reactor.

[illegible] more practical definition of the [illegible] be given in terms of neutron [illegible]

[illegible] production in the [illegible] neutron loss [illegible]

[illegible] that if λ=1, the number of [illegible] generations will be the same [illegible] will be time-independent. We [illegible]

[illegible] by $\lambda = 1$ as being critical. Hence the [illegible] of the nuclear engineer is to design the [illegible] critical. One possible approach would be to [illegible] reactor 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] of the core composition is through [illegible] control poison density without which the [illegible] critical thus allowing for a margin of error [illegible] and more importantly for reasonably long [illegible]

[illegible] CROSS SECTION DATA

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

a. [illegible] resulting from the collision between [illegible] particles.

b. [illegible] disintegrations of nuclei.

[illegible] neutron-nucleus collision events involved [illegible] are an example of the first type of [illegible] reactions depend not only on the [illegible] particles, as in the case of the [illegible] also the relative velocity with which [illegible] An example of the second type of [illegible] decay of fission products, since [illegible] unstable.

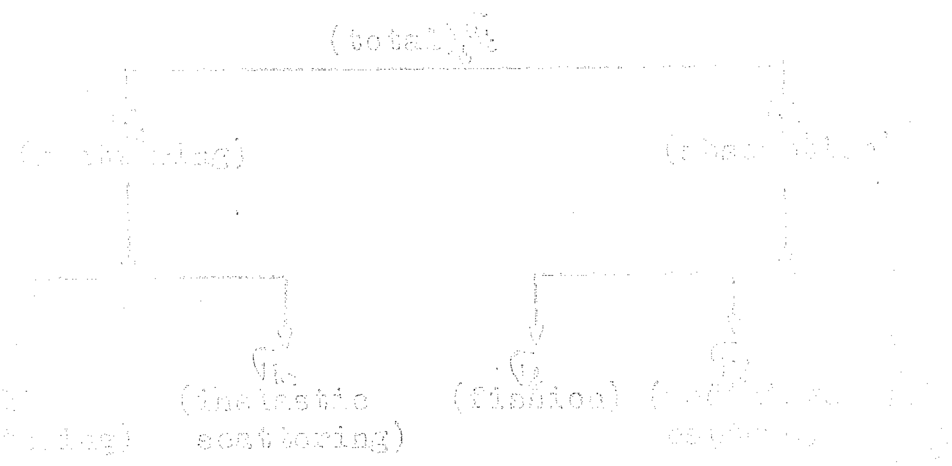
[illegible] wide variety of possible nuclear [illegible] of interest in the analysis of [illegible] involve interactions between [illegible] that a neutron-nucleus interaction [illegible] by nuclear cross sections. [illegible] and the geometrical cross [illegible] of the order of 10^{-24} cm². [illegible] nuclear cross sections would [illegible] cm². However this [illegible] cross section can frequently be [illegible] larger or smaller than the geometrical [illegible] the nucleus due to resonance effects which [illegible] of quantum mechanical nature of the [illegible] system. For example, the [illegible]

[illegible] for slow neutrons is almost one million [illegible] geometrical cross section.

[illegible] such cross sections can be used to [illegible] nuclear reaction, thus the definition [illegible] cross sections for each type of neutron-nuclear [illegible] and for different nuclei. For example, cross sections [illegible] absorption and scattering are denoted by [illegible]. Finally, we can introduce the [illegible] related to the probability that any [illegible] reaction will occur. Obviously

$$\sigma_t = \sigma_s + \sigma_a = \sigma_e + \sigma_{in} + \sigma_f + \sigma_\gamma + \sigma_{n\alpha} + \cdots$$

[illegible] diagram of the hierarchy of cross sections [illegible] conventional notation is shown in Figure [illegible]



[illegible] III-4 Neutron cross section [illegible]

[illegible] we have defined the concept of a [illegible] introducing the neutrons having [illegible] incident upon the target nucleus. [illegible] that such cross sections [illegible] neutron speed or energy [illegible] cross sections for nuclear [illegible] observed, a very strong energy [illegible] of the neutron cross section [illegible] usually much weaker and [illegible] reactor applications.

[illegible] LIBRARY SET

[illegible] microscopic cross section tape for this [illegible] various codes but, GELS, developed by K.P.N. [illegible] SCRUGS under the auspices of GKSS (Gesellschaft [illegible] Kernenergieverwertung in Schiffbau und Schiffahrt [illegible] specifically for this purpose.

[illegible] calculation of the actual microscopic cross [illegible] necessary to divide the energy spectrum into [illegible] is divided into 45 micro groups and [illegible] data for all the micro groups are supplied [illegible] micro groups can be condensed up to 15 [illegible] group data is generated by GELS for [illegible] 15 in the present version of [illegible] is stored in the NGRLS file and [illegible] parameter LIBRA. Thus, it is possible [illegible] sets of microscopic cross section [illegible] library set is outlined in Figure [illegible] to assign each initial composition [illegible]

[illegible] library set number (NBL) is greater than 1, [illegible] supplied consecutively by the [illegible] distinctive number, called [illegible] to the order in which such sets appear [illegible]

[illegible] SELF SHIELDING SET

[illegible] reactor core is not homogeneous [illegible] within a zone is uniform. The flux [illegible] increases that is flux dependent [illegible] uniform $\Sigma_a(L,IG)$; such [illegible] absorption and other [illegible] therefore effective group [illegible] actual constants with [illegible] called the self shielding [illegible]

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

[illegible] possible, in KREBUS, to specify [illegible] self shielding sets [illegible] each initial composition to a [illegible]

[illegible]	Isotope Index	Nuclear data for [illegible]		
	1	σ_{tr}^{i} σ_{a}^{i} σ_{f}^{i} σ_{s}^{i} $\nu\sigma_{f}^{i}$ e^{i} $f^{i\to j}$ $\sigma_{s}^{i\to j}$	$i=1,2,\ldots,NG$ $i=1,2,\ldots,NG$ $i=1,2,\ldots,NG-1$ $i=1,2,\ldots,NG$ $i=1,2,\ldots,NG$ $i=1,2,\ldots,NG$ $j=i+1,\ldots,$ [illegible] $j=1,2,\ldots,NG \quad j\neq i$ $i=1,2,\ldots,NG$	only for [illegible]
	2	σ_{tr}^{i} σ_{a}^{i} σ_{f}^{i} . . .		
		σ_{tr}^{i} σ_{a}^{i} . . .		
[illegible]	[illegible]	σ_{tr}^{i} . . .		

[illegible] Schematic representation of [illegible]

[illegible] set, the specification of one self shielding [illegible] to one generic self shielding set. If [illegible] shielding set (NBS>1) are present as many [illegible] consecutively. Each set will take a [illegible] (called the set number) according to [illegible] sets appear in the input deck.

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

[illegible] must have NG cards, one for each [illegible] with the self shielding coefficient [illegible] sum to the total number of self [illegible] such that

$$[illegible]\ NG.NGP.\sum_{K=1}^{NBS} NBT(K) \leq KCOF$$

[illegible] present version of EREBUS

[illegible] = 4000

[illegible] of the subroutine LIBRA is to read [illegible] the input data. If it gives any [illegible] execution is discontinued.

[illegible] microscopic nuclear data and self shielding [illegible] for use in the calculation of [illegible] the those group constants [illegible] in the calculation of the [illegible] and eventually in [illegible] will be [illegible] of course, [illegible]

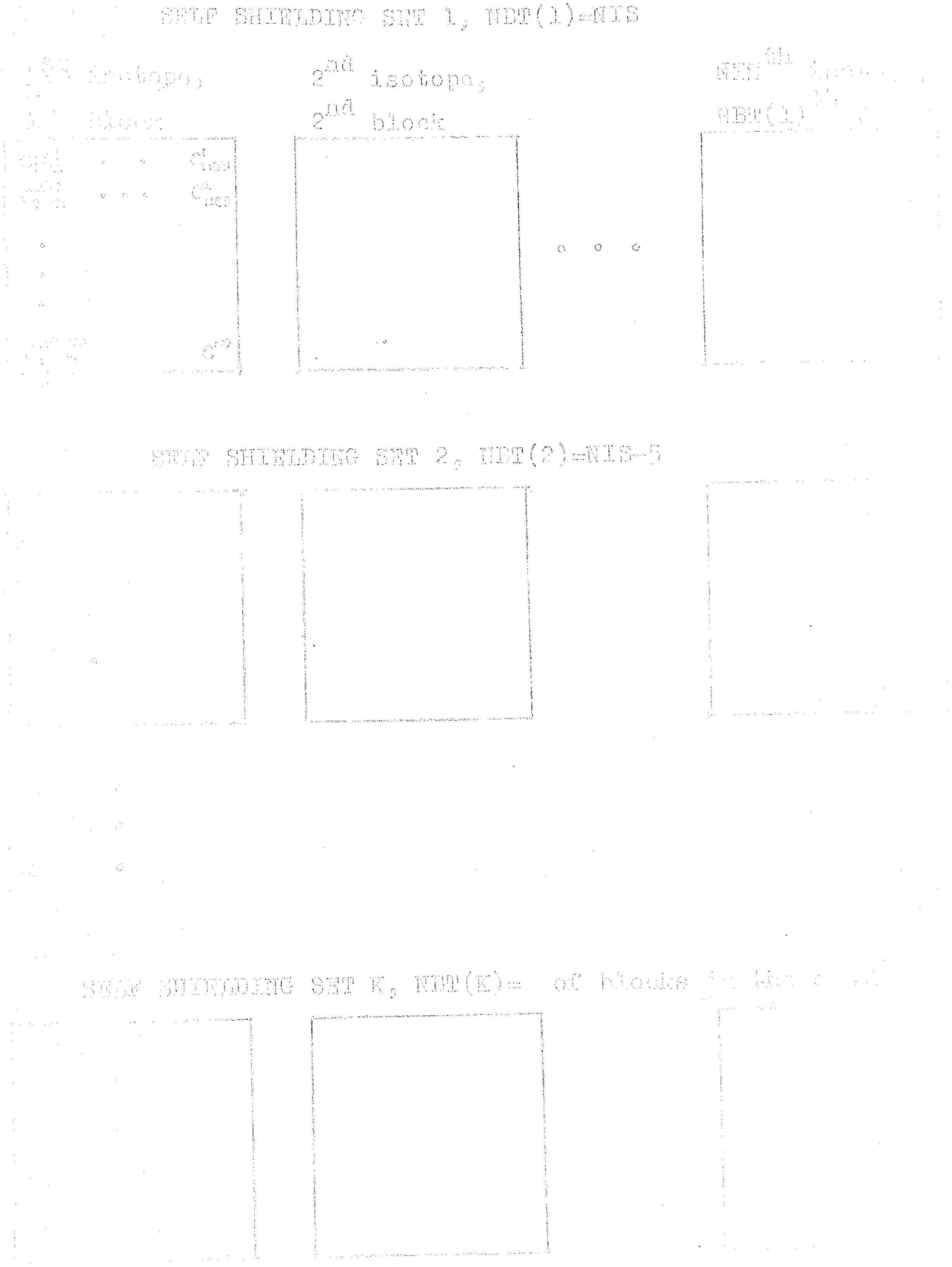


Figure III.6 Schematic representation of self shi [illegible]

CHAPTER-IV

The product of the atomic number density N and the [illegible] section σ_t is denoted by Σ_t. It is called [illegible] section

$$\Sigma_t = N\sigma_t = \frac{\#}{cm^3} \cdot cm^2 = cm^{-1} \qquad (IV.1)$$

[illegible] Σ_t as the total macroscopic cross section [illegible] target material, whereas the microscopic [illegible] the probability of interaction with [illegible] It should be noted that Σ_t is not really [illegible], since its unit is inverse length.

[illegible] discussion has been restricted to total [illegible] characterize the probability that a [illegible] type of reaction. We can generalize this [illegible] defining the macroscopic cross section for [illegible] as the microscopic cross section for [illegible] multiplied by the number density N [illegible] of interest. For example, the macroscopic [illegible] would be defined as

$$\Sigma_f = N\sigma_f$$

[illegible] of a macroscopic cross section can [illegible] homogeneous mixtures of different [illegible] homogeneous mixture of three [illegible] Y, and Z, with respective atomic [illegible] and self shielding factors ξ_x, ξ_y [illegible] cross section [illegible]

$$\Sigma_t = N_x\xi_x\sigma_t^x + N_y\xi_y\sigma_t^y + N_z\xi_z\sigma_t^z$$

[illegible] σ_t^x is the microscopic cross section for nuclide [illegible]

[illegible] neutron-nuclear reaction cross sections [illegible] energy of the incident neutron.

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

$$\sum(r, E, t) = N(r,t)\sigma(E) \qquad \text{(IV. [illegible])}$$

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

In the next two sections, first the number densities of [illegible] [illegible] after that, macroscopic cross sections [illegible] [illegible].

[illegible] SUBROUTINE SETUP

[illegible] number densities of burnable isotopes, [illegible] [illegible] group constants, are read from the [illegible] [illegible] the variable IND = 0. These number densities [illegible] [illegible] unit number 10 initially as input and [illegible] [illegible] results for the following time steps.

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

$$W(L,J) = \frac{N(L,J).V(L).A(J)}{Av.} \qquad \text{(IV. [illegible])}$$

where

J = Burnable (time dependant) isotope

N(L,J) = number density of the J^{th} isotope in region L [illegible]

V(L) = Volume of the L^{th} region (cm^3)

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

Av = Avogadro number (#/cm^3)

W(L,J) = Weight of the J^{th} burnable isotope in region L [illegible]

When IND = 2 the same calculation is made to [illegible]

[illegible] of burnable isotopes in composition M.

$$W(M,J) = \sum_{L} \frac{N(L,J).V(L).A(J)}{Av.} \qquad (IV.[illegible])$$

[illegible] composition M consists of regions denoted by [illegible] L.

[illegible] calculates the total weight of each burnable isotope, [illegible] in grams.

$$W(J) = \sum_{L=1}^{NREG} \frac{N(L,J).V(L).A(J)}{Av.} \qquad (IV [illegible])$$

[illegible] on a tape file the data required for a [illegible] microscopic nuclear data, bucklings, [illegible] coefficients, and number densities.

[illegible], if there is fuel shuffling, then the [illegible] of the burnable isotopes in the region L are [illegible] other region or composition. Clearly fuel shuffling [illegible] considered only if the time step number is [illegible]

[illegible] fuel shuffling has been effected then a new fuel [illegible] in which case the subprogram calculates [illegible] of the isotopes in each region and for each [illegible]

[illegible] SUBROUTINE SERCON AND MAPPIO

[illegible] determining the type of the criticality [illegible] and the type of start, this subprogram calls [illegible] the condition of the reactor core; one indicating [illegible] and the other doing the same for [illegible]

[illegible] in the criticality searches, [illegible] calculates the self shielding [illegible] and prints out the latter.

[illegible] can solve, at each time step, four types of [illegible]. These are classified as follows;

[illegible] STRAIGHT DIFFUSION CALCULATION

[illegible] the solution of the diffusion [illegible]

[illegible] the eigenvalue λ, which is coincident with the multiplication factor k_{eff} of the reactor. This type of calculation [illegible] called "Straight Burnup".

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

This is the search of a prefixed multiplication factor [illegible] by a uniform variation of a control isotope number density [illegible]. The number density of the control isotope [illegible] input for each region, except for a multiplicative [illegible] the dilution factor, unique for the whole reactor [illegible] to be calculated by the program. Maximum and minimum values [illegible] Θ_{max} and Θ_{min} are to be inputted. The [illegible] given as input.

The program first determine the eigenvalues [illegible] corresponding to Θ_{max} and Θ_{min}. If $\lambda_1-\lambda_c$ and $\lambda_2-\lambda_c$ have different signs, the first estimate $\Theta^{(1)}$ is determined by linear interpolation [illegible]

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

[illegible] process is carried out, by successive linear [illegible] between two consecutive couples of λ and Θ, until [illegible] $\Theta^{(T)}$ is found such that:

$$\left|\lambda^{(T)}-\lambda_c\right| < \eta \qquad [illegible]$$

[illegible] is set equal to $\Theta^{(T)}$ and the search is terminated.

If the reactivity $\delta\lambda$ does not change sign [illegible] the critical search is interrupted, and [illegible] the final edits of a normal problem (neutron [illegible] and composition integrals) corresponding [illegible] time step.

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

[illegible] list of regions is given in input. The [illegible] one or more in such a list. One or more [illegible] list can be grouped, and such group [illegible]. A control bank can consist of a single [illegible]

[illegible] control isotope is changed simultaneously in all [illegible] belonging to the same control bank, therefore [illegible] and minimum values, N_{max} and N_{min}, of the [illegible] density, must be supplied for any of the [illegible]

[illegible] suppose now that, following the given control [illegible] is examining a given control bank. The program [illegible] the eigenvalues λ_1 and λ_2 corresponding [illegible] If the reactivity $\delta\lambda = \lambda_1 - \lambda_2$ does change sign [illegible] to N_{min}, the critical value N_c is determined [illegible] by consecutive linear interpolations, along [illegible] described for the determination of the [illegible]

[illegible] contrary, the reactivity $\delta\lambda$ does not [illegible] the criticality cannot be achieved [illegible] under examination, the program goes on [illegible] control banks, as indicated by the control [illegible]

[illegible] the control list is exhausted, the critical [illegible] and the problem ends with the final [illegible] step. Regarding the number densities of [illegible] the regions not belonging to the control [illegible] examination, the following rules hold:

[illegible] control banks, which include the given [illegible] bank under examination, the control [illegible] in this region takes the value N_{min} of the [illegible] region appears;

[illegible] all control banks, which include the given [illegible] bank under examination, the number density [illegible] the value N_{max} of the first bank in [illegible]

[illegible] of the control banks, including [illegible] the other ones follow the bank under [illegible] density in this region takes the [illegible] the preceding banks.

[illegible] like to point out that, with regard [illegible] region appears in more than [illegible] the N_{max} in one bank should be [illegible] in order to make sense from a physical [illegible]

[illegible] BOUNDARY SEARCH

[illegible] is the search of a prefixed multiplication factor λ [illegible] means of a quasi-continuous movement of the boundary of [illegible] [illegible] areas, of rectangular shapes.

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

[illegible] displacement of the moving boundary from one [illegible] [illegible] upper one, constitutes "an elementary step" [illegible] [illegible] search is performed in a fashion quite [illegible] [illegible] one (type iii). A list of control areas [illegible] [illegible] they are grouped into control banks, and the [illegible] [illegible] all control areas belonging to a bank are [illegible] [illegible]. Therefore, an upper and lower limit, [illegible] [illegible] also be specified for each bank, within which [illegible] [illegible] boundary is confined.

[illegible] suppose now that, following the given control [illegible] [illegible] is examining a given control bank. The [illegible] [illegible] moving boundary of each region of the bank [illegible] [illegible]. Successively the boundary is [illegible] [illegible] at a time, and at each "elementary step" the [illegible] [illegible] evaluated.

[illegible] search is considered completed when a position of [illegible] [illegible] is reached, such that either the [illegible] [illegible] or the reactivity $\delta\lambda = \lambda - \lambda_c$ does change sign [illegible] [illegible] positions of the moving boundary.

In the last case, the critical boundary is [illegible] [illegible] which gives the smaller reactivity.

[illegible] the moving boundary comes to the upper limit [illegible] [illegible] neither of the two conditions stated above, [illegible] [illegible] execute the same procedure for the next [illegible] [illegible]

[illegible] the position of the moving boundary [illegible] [illegible] belonging to the one under the [illegible] [illegible] holds:

[illegible] all control banks, including the given [illegible] [illegible] bank under consideration, the moving boundary [illegible] [illegible] lower limit y[illegible] of the last bank in which [illegible] [illegible]

c. If all control banks, including the given area, fol[illegible] under examination, the moving boundary of this area is [illegible] at the lower limit y_{max} of the first bank in which such a[illegible] [illegible]

d. If some of the control banks, including the given area, [illegible] and the other ones follow the bank under examination, the [illegible] boundary of this area is set at the upper limit y_{max} of the [illegible] of the preceding banks.

Figure IV-1 shows a reactor with 5 control areas. The first bank is constituted by areas 1, 2, 3, the second one by 3, 4, 5. In this case the control list is: 1, 2, 3, 3, 4, 5. The [illegible] are represented by the shadowed zones.

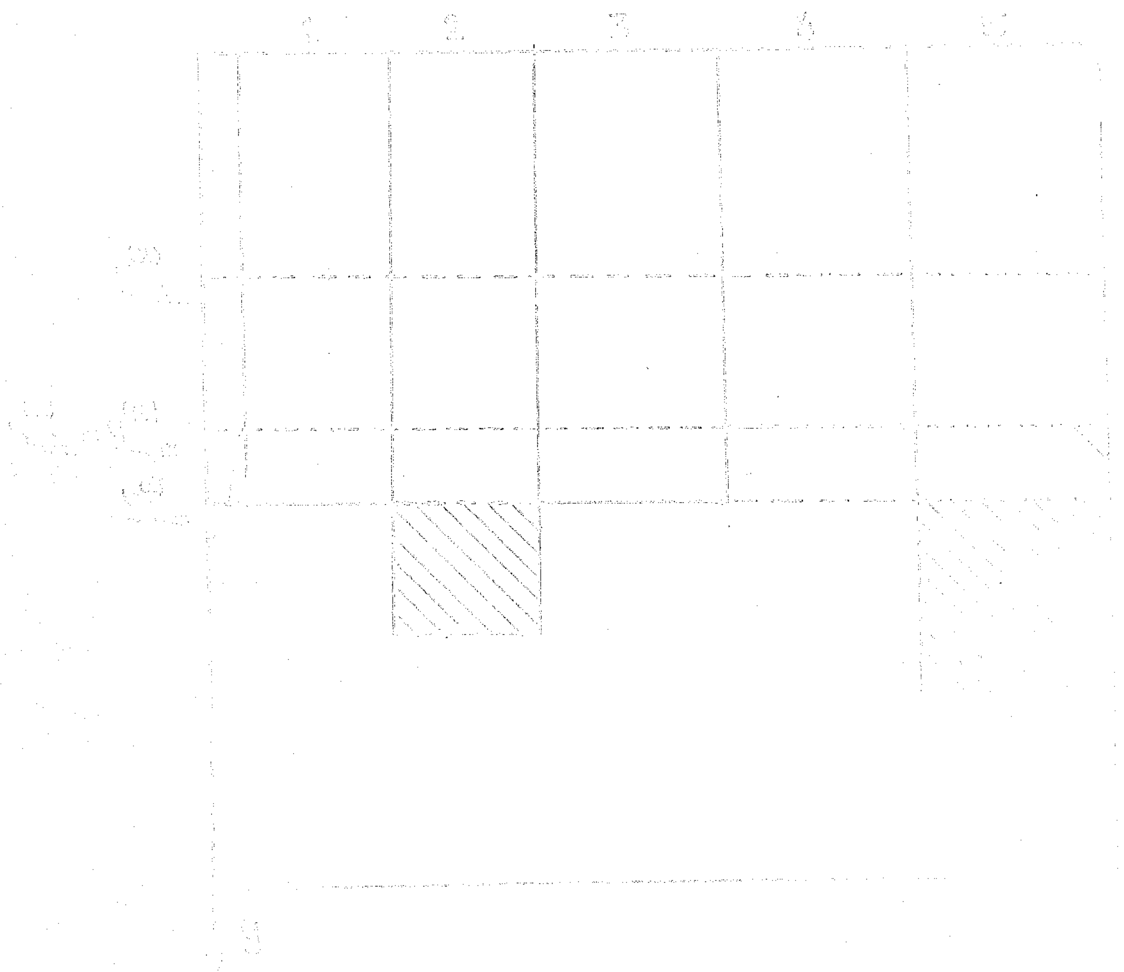


Figure IV-1 Example of control areas

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-B-ii, iii and iv (in the boundary search (iv), an iteration is constituted by an "elementary step" of the moving 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 ρ, in paragraph (ii) does not change sign going from ρ_{max} to ρ_{min}.

b) Outer iterations: They are defined in the same way they generally are in most diffusion programs; the outer iterations are characterized by the successive estimates of the fission neutron source and the eigenvalue λ, keeping fixed [illegible] the [illegible] reactor configuration.

Two criteria are employed to cease the outer iterations:

1) The eigenvalue convergence

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

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

2) The pointwise convergence

$$\frac{\lambda^{(t)}_{max}-\lambda^{(t)}_{min}}{\lambda^{(t)}} < \delta \qquad (IV-11)$$

where δ is an input "pointwise convergence criterion".

In every criticality iteration, the outer iterations are interrupted when condition (IV-10) is fulfilled. Only when the criticality search condition (IV-9) is achieved (or an equivalent in the boundary search), the outer iterations are continued until the pointwise condition (IV-5) is fulfilled. This last condition is considered even if the criticality search has been stopped by causes (2), (3), (4). If the search has been stopped by cause (1), the problem ends neither satisfying (IV-10) nor (IV-11). The outer iterations [illegible]

[illegible] when the pointwise criterion (IV-11) is fulfilled.

[illegible] Inner iterations: The inner iterations are performed [illegible] [illegible] of a given outer iteration in order to calculate [illegible] group fluxes corresponding to the fission source of [illegible] [illegible].

The calculation of type of straight burnup is performed with [illegible] outer iterations only.

[illegible] – CALCULATION OF THE SELF SHIELDING FACTORS

For the calculation of effective group constants, [illegible] necessary to generate self shielding factores it was stated in Chapter III-D.3.

Self shielding factors $\xi^{i,j,l}$ are automatically calculated [illegible] at each time step by the semi-empirical formula

$$\xi^{i,j,l} = g^{i,j}\left(X^{i,j,l}\right) \qquad [illegible]$$

with

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

The function $g^{i,j}(z)$ is given according to an option [illegible] [illegible] of the following expressions. If the isotope [illegible] [illegible] ISHZ(J) equals two or three, then the expression [illegible] [illegible]:

$$g^{i,j}(z) = \sum_{n=0}^{n} C_n^{i,j} z^n \qquad [illegible]$$

[illegible] ISHZ(J) equals zero or one, then the following [illegible] is used:

$$g^{i,j}(Z) = \frac{C^{i,j}}{\sqrt{1 + \sum_{n=1}^{m} C_n^{i,j} Z^n}} \qquad [illegible]$$

where the independent variable is given according to another [illegible] tion by either of the following expressions:

If [illegible](J) equals zero or two, then

$$X^{i,j,l} = \sum_{j\in l}^{J} N^{j,l} \left(\sigma_a^{i,j} + \sigma_r^{i,j} \right) \qquad \text{(IV-[illegible])}$$

or, if [illegible](J) equals one or three

$$X^{i,j,l} = N^{j,l} \qquad \text{(IV-[illegible])}$$

The meaning of the symbols are as follows:

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

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

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

The isotopes included in the summation (IV-1[illegible]) are specified in input. The coefficient $C_K^{i,j}$ and the above microscopic cross sections are input data, and are generally group and isotope [illegible].

IV-2-4 CALCULATION OF THE GROUP CONSTANTS

The reason we would like these diffusion parameters [illegible] to use this information in the calculation of the [illegible] of the finite difference equations and eventually [illegible] figure the criticality of a reactor. The group constants [illegible] calculated in this subprogram.

We have briefly discussed the macroscopic cross sections and group constants in Chapter IV.

If variable index IDD=1, then the diffusion coefficient [illegible] macroscopic cross sections, except the scattering matrix, [illegible] by the subprogram SERCON. Group constans are [illegible] all isotopes. Thus, they would be defined as:

$$\Sigma_a^{i,l} = \sum_{j=1}^{NI} N^{j,l}\, \xi^{i,j,l}\, \sigma_a^{i,j}$$

Macroscopic absorption cross section [illegible] (cm^{-1})

In a similar fashion we can define

$$\Sigma_f^{i,l} = \sum_{j=1}^{NI} N^{j,l}\, \xi^{i,j,l}\, \sigma_f^{i,j}$$ Macroscopic fission cross section (cm^{-1}) (IV-18)

and

$$\nu\Sigma_f^{i,l} = \sum_{j=1}^{NI} \nu N^{j,l}\, \xi^{i,j,l}\, \sigma_f^{i,j}$$ Macroscopic nu-fission cross section (cm^{-1}) (IV-19)

and

$$\Sigma_r^{i,k,l} = \sum_{j=1}^{NI} N^{j,l}\, \xi^{i,j,l}\, \sigma_r^{i,j}$$ Macroscopic removal cross section from group i to k (cm^{-1}) (IV-20)

and

$$E_f^{i,l} = \sum_{j=1}^{NI} N^{j,l}\, \xi^{i,j,l}\, \sigma_f^{i,j}\, e^{i,j}$$ Macroscopic cross-section for energy production (J/cm) $e = 3.2 \times 10^{-11}$ J (IV-21)

and

$$\Sigma_{tr}^{i,l} = \sum_{j=1}^{NI} N^{j,l}\, \xi^{i,j,l}\, \sigma_{tr}^{i,j}$$ Macroscopic transport cross section (cm^{-1}) (IV-22)

and

$$D^{i,l} = \frac{1}{3\sum_{j=1}^{NI} N^{j,l}\, \xi^{i,j,l}\, \sigma_{tr}^{i,j}}$$ Diffusion coefficient (cm) (IV-23)

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

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

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

[illegible]

[illegible] collects the Σa, Σr and $D \times B^2$ which signify the [illegible] terms, [illegible] terms, diffusion coefficient and nu-fission and [illegible] them on logical unit 4.

If the variable index IND=2, then the program calculates the removal 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 restart.

Let us consider how one could attempt to solve the neutron diffusion equation directly by the aid of a digital computer. Since the advantage of using a computer is its ability to solve 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 "discretising" each of the terms in the diffusion equation, that is, by replacing functions of continuous variables by a discrete set of values at a discrete set of mesh grid points. The derivatives and integrals appearing in the diffusion equation must also be replaced by a corresponding discrete representation. In this way one arrives at a set of algebraic equations for the discrete representation of the dependent 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 [illegible] represented by a two dimensional map; the axes of the map are either x-y or r-z or r-θ. To simplify the description, we will consider the x-y geometry in detail. It is not difficult to see how the x-y case can be extended to the r-z or r-θ geometries.

The mesh system is defined as shown in figure V-1 by vertical and horizontal lines. In this system, each rectangle is termed a mesh square. Considering the numerical solution of the more general diffusion equation;

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

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

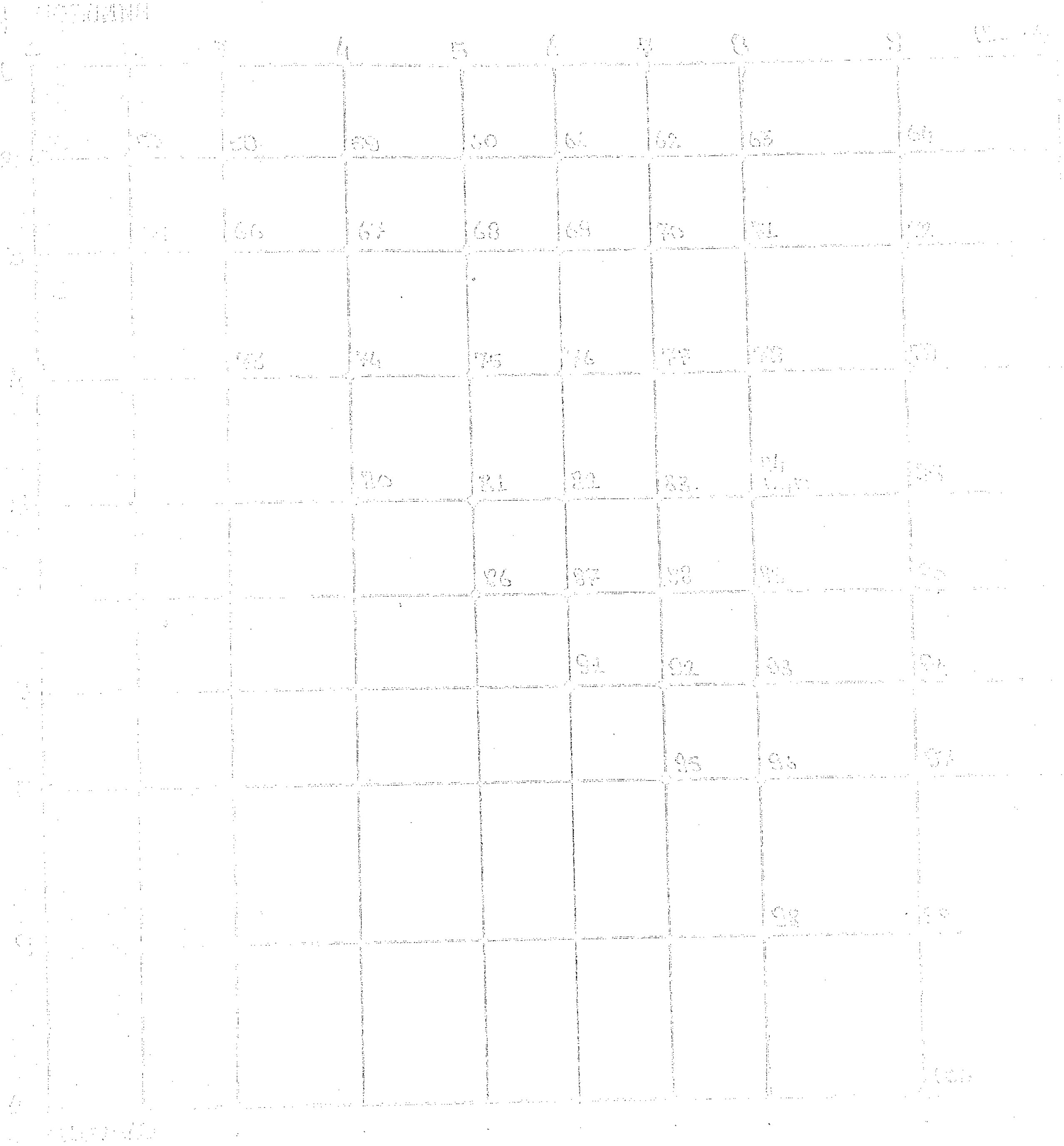


Figure 7.1. The complete x-y mesh

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 types of volumes around the mesh point (m,n). These volumes are illustrated in Figure V-2. Each volume may or may not have different group constants, or different region indices; since interfaces are always taken to be mesh points.

Subprogram CODI calculates v_1, v_2, v_3, and v_4 that are the volumes indicated in Figure V-2.

$$v_1 = \frac{\Delta x_2 \cdot \Delta y_1}{4}, \quad v_2 = \frac{\Delta x_1 \cdot \Delta y_1}{4}, \quad v_3 = \frac{\Delta x_1 \cdot \Delta y_2}{4}, \quad v_4 = \frac{\Delta x_2 \cdot \Delta y_2}{4}$$

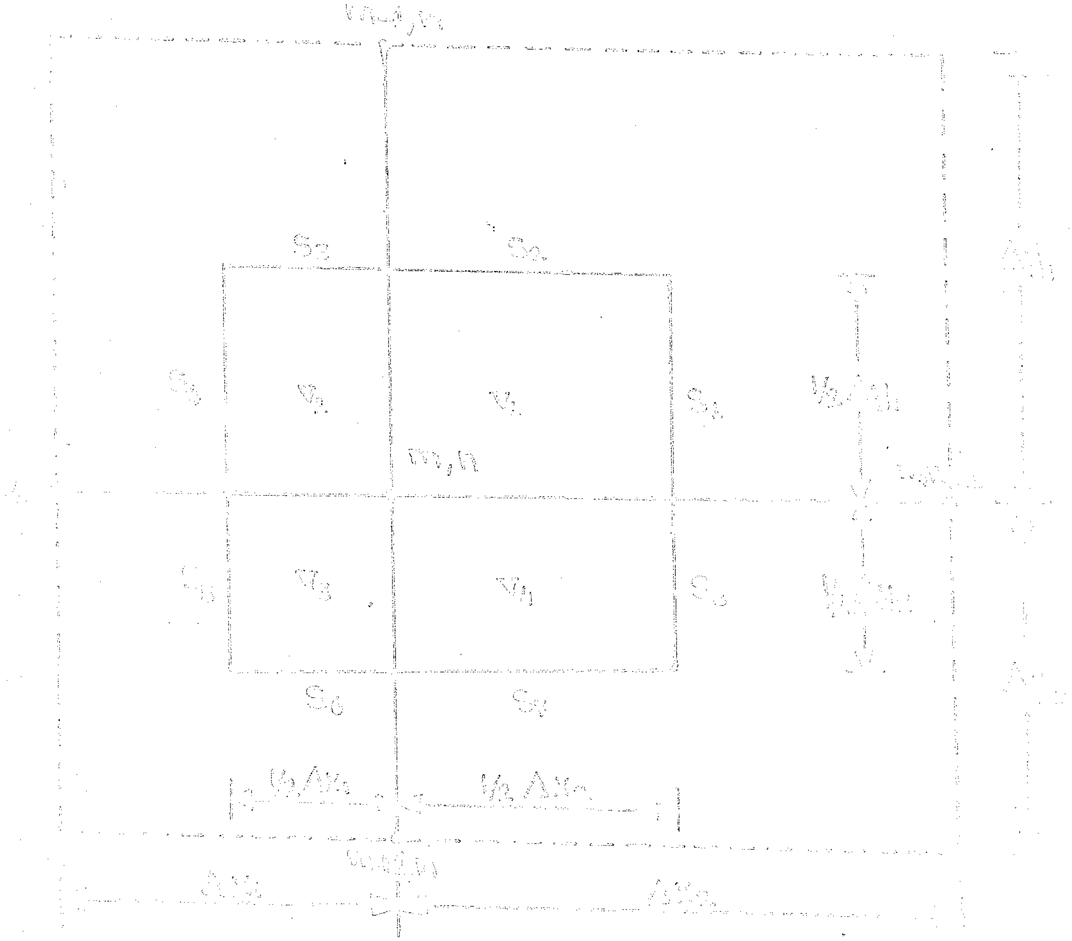


Figure V-2 Part of the mesh shown in detail.

Reactor regions have been described in subprogram SIMDAC, so 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. Each mesh point number describes a different mesh square.

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

V-7 COEFFICIENTS OF THE FINITE DIFFERENCE EQUATIONS

The difference equations are obtained by integrating the diffusion equation over the four rectangular volumes associated with the mesh point (m,n)

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

(V-[illegible])

Consider each term separately. The first integral is along the surface of the region of integral and $\partial/\partial n$ is the derivative normal to the surface;

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

(V-[illegible])

In performing the surface integral of the right side of Equation (V-[illegible]), we approximate the derivative by

$$\frac{d\phi^i}{dx} = \frac{\phi^i_{m+1,n}-\phi^i_{m,n}}{\Delta x_m}$$ on the surface S_1 and [illegible] (V-[illegible])

$$\frac{d\phi^i}{dy} = \frac{\phi^i_{m,n+1}-\phi^i_{m,n}}{\Delta y_n}$$ on the surface [illegible] and [illegible] (V-[illegible])

$$\frac{d\phi^i}{dx} = \frac{\phi^i_{m-1,n}-\phi^i_{m,n}}{\Delta x_{m-1}}$$ on the surface S_4 and [illegible] (V-[illegible])

$$\frac{\partial\phi^i}{\partial y} = \frac{\phi^i_{m+1,n}-\phi^i_{m,n}}{\Delta y_2} \qquad \text{on the surface } S_6 \text{ and } S_7 \qquad \text{(V-7)}$$

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

$$-\int_S D^i(x,y)\nabla\phi^i(x,y)\,dS = -D^i_1\,\frac{\phi^i_{m,n}-\phi^i_{m-1,n}}{\Delta y_1}\cdot\frac{\Delta x_2}{2} - D^i_2\,\frac{\phi^i_{m,n}-\phi^i_{m-1,n}}{\Delta y_1}\cdot\frac{\Delta x_1}{2}$$

$$= \frac{D^i_1\Delta x_2 + D^i_2\Delta x_1}{2\,\Delta y_1}\left(\phi^i_{m,n}-\phi^i_{m-1,n}\right) \qquad \text{(V-8)}$$

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

$$\frac{[illegible]\Delta y_1 + [illegible]\Delta y_2}{2\Delta x_{[illegible]}}\left(\phi^i_{m,n}-\phi^i_{m,n-1}\right) \qquad \text{along } S_2 \text{ and } S_4 \qquad \text{(V-9)}$$

$$\frac{[illegible]\Delta x_{[illegible]} + [illegible]\Delta x_{[illegible]}}{2\Delta y_2}\left(\phi^i_{m,n}-\phi^i_{m+1,n}\right) \qquad \text{along } S_5 \text{ and } S_7 \qquad \text{(V-10)}$$

$$\frac{[illegible]\Delta y_{[illegible]} + [illegible]\Delta y_{[illegible]}}{2\Delta x_2}\left(\phi^i_{m,n}-\phi^i_{m,n+1}\right) \qquad \text{along } S_6 \text{ and } S_8 \qquad \text{(V-11)}$$

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

The second integral becomes

$$\int_S \Sigma^i_r(x,y)\phi^i(x,y)\,dS = \left(\Sigma^i_{r1}\cdot V_1 + \Sigma^i_{r2}\cdot V_2 + \Sigma^i_{r3}\cdot V_3 + \Sigma^i_{r4}\cdot V_4\right)\phi^i_{m,n}$$

$$= \sum_{k=1}^{4}\left(\Sigma^i_{rk}\cdot V_k\right)\cdot\phi^i_{m,n} \qquad \text{(V-12)}$$

where Σ^i_{rk} is the value of $\Sigma^i_r(x,y)$ in the volume represented by V_k (k=1,2,3,4). Similarly the first term on the right side of Equation (V-2) becomes

$$\frac{\chi^i\nu}{\lambda}\sum_{j=1}^{NG}\int_S \Sigma^j_f(x,y)\phi^j(x,y)\,dS = \frac{\chi^i\nu}{\lambda}\sum_{j=1}^{NG}\left(\Sigma^j_{f1}V_1+\Sigma^j_{f2}V_2+\Sigma^j_{f3}V_3+\Sigma^j_{f4}V_4\right)\phi^j_{m,n}$$

$$= \frac{\chi^i\nu}{\lambda}\sum_{j=1}^{NG}\sum_{k=1}^{4}\Sigma^j_{fk}\cdot V_k\,\phi^j_{m,n} \qquad \text{(V-13)}$$

where $\bar{\Sigma}^i_{fk}$ is the value of $\Sigma^i_f(x,y)$ in the volume represented by V_k. The second integral on the right side of Equation (V-2) becomes

$$\sum_{\substack{j=1\\ j\neq i}}^{NG}\int_S \Sigma^{j\to i}_R(x,y)\,\phi^j(x,y)\,dS = \sum_{\substack{j=1\\ j\neq i}}^{NG}\left(\Sigma^{j\to i}_{R1}\cdot V_1+\Sigma^{j\to i}_{R2}\cdot V_2+\Sigma^{j\to i}_{R3}\cdot V_3+\Sigma^{j\to i}_{R4}\cdot V_4\right)\phi^j_{m,n}$$

$$= \sum_{\substack{j=1\\ j\neq i}}^{NG}\sum_{k=1}^{4}\Sigma^{j\to i}_{Rk}\cdot V_k\cdot\phi^j_{m,n} \qquad (V-14)$$

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

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

$$S^i_{m,n} = \frac{\chi^i}{\lambda}\sum_{j=1}^{NG}\sum_{k=1}^{4}\nu\Sigma^j_{fk}V_k\phi^j_{m,n} + \sum_{\substack{j=1\\ j\neq i}}^{NG}\sum_{k=1}^{4}\Sigma^{j\to i}_{Rk}\cdot V_k\cdot\phi^j_{m,n}$$

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

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

$$+e^i_{m,n}\phi^i_{m,n-1}=S^i_{m,n}$$

where the coefficient are;

$$a^i_{m,n} = \sum_{k=1}^{4}\Sigma^i_{tk}V_k-\left(b^i_{m,n}+c^i_{m,n}+d^i_{m,n}+e^i_{m,n}\right)$$

$$b^i_{m,n} = -\frac{D^i_1\Delta x_1 + D^i_2\Delta x_2}{2\Delta y_2}$$

$$c^i_{m,n} = -\frac{D^i_4\Delta x_2 + D^i_3\Delta x_1}{2\Delta y_1}$$

$$d^i_{m,n} = -\frac{D^i_1\Delta y_1 + D^i_4\Delta y_2}{2\Delta x_1}$$

$$d^{i}_{m,n} = -\frac{D^{i}_{k}\Delta y_{l} + D^{i}_{j}\Delta y_{m}}{2\Delta x_{i}} \qquad (V-21)$$

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 $\Sigma^{i}_{a} \geq 0$. Notice also the symmetry properties $b^{i}_{m,n} = c^{i}_{m,n}$ and $d^{i}_{m,n} = e^{i}_{m,n}$.

V-2 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

$$D\frac{\partial}{\partial n}\phi(s) + \gamma(s)\,\phi(s) = 0 \qquad (V-22)$$

where s is the coordinate along the boundary; then

$$\gamma(s) = \frac{\alpha}{\beta} \qquad (V-23)$$

The boundary condition at the edge of the reactor core is

$\phi(x,y)=0$ for m=1 or M=NPY (V-24)

$\phi(x,y)=0$ for n=1 or N=NPX (V-25)

An alternative set of boundary conditions could be;

$$\beta(x,y)\,D(x,y)\frac{\partial\phi(x,y)}{\partial x} + \alpha(x,y)\,\phi(x,y) = 0 \qquad (V-26)$$

$$\beta(x,y)\,D(x,y)\frac{\partial\phi(x,y)}{\partial y} + \alpha(x,y)\,\phi(x,y) = 0 \qquad (V-27)$$

Consider one particular outer boundary, for example, the left boundary m=1. If the condition, in Equation (V-24) prevails, we simply set φ equal to zero for all n. If the condition is in Equation (V-26), then we integrate the diffusion equation over the volumes v_2 and v_3. The contributions for v_1 and v_4 are now zero, because they now don't exist. The contributions from the surfaces S_3, S_4, S_5, and S_6 are the same as before. [illegible] S_1, S_2, S_7, and S_8 don't exist for this boundary point. However, we have two 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 of $\phi^i(x,y)$ 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:

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

$$= -\left(\frac{\gamma_1^i\,\Delta y_1}{2} + \frac{\gamma_8^i\,\Delta y_2}{2}\right)\phi^i_{n,j} \qquad [illegible]$$

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

The surface integrals along S_4 and S_5 become:

$$\frac{D^i\Delta x + D^i\Delta y_2}{2\Delta x_1}\left(\phi^i_{n,j} - \phi^i_{n,j-1}\right) \qquad [illegible]$$

and along S_3

$$\frac{D^i\Delta x}{\Delta y}\left(\phi^i_{n,j} - \phi^i_{n-1,j}\right) \qquad [illegible]$$

and along S_6

$$\frac{D^i\Delta y_2}{\Delta y_2}\left(\phi^i_{n,j} - \phi^i_{n+1,j}\right) \qquad [illegible]$$

The contribution for v_2 and v_3 are unchanged. [illegible] in Equation (V-2) apply only to v_2 and v_3, so that the [illegible] right side of Equation (V-2) become [illegible]

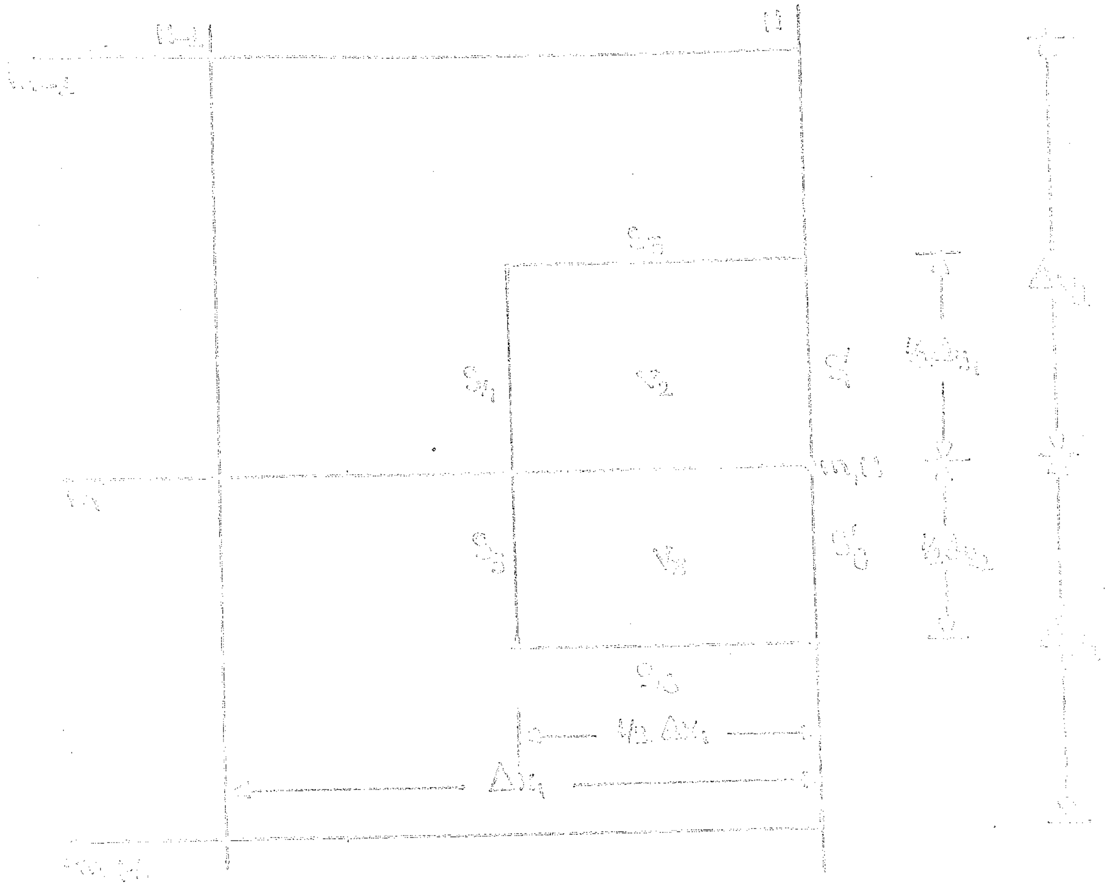


Figure V.3 Area of integration near the outer boundary.

$$\int \Sigma^i_t(x,y)\,\phi(x,y)\,dx\,dy = \left(\Sigma^i_{t2}\cdot v_2 + \Sigma^i_{t3}\cdot v_3\right)\phi^i_{m,N}$$ (V-[illegible])

$$\frac{\chi^i\nu}{\lambda}\sum_{j=1}^{NG}\int \Sigma^j_f(x,y)\,\phi^j(x,y)\,dx\,dy = \frac{\chi^i\nu}{\lambda}\sum_{j=1}^{NG}\left(\Sigma^j_{f2}\cdot v_2 + \Sigma^j_{f3}\cdot v_3\right)\phi^j_{m,N}$$ (V-[illegible])

$$\sum_{\substack{j=1\\ j\neq i}}^{NG}\int \Sigma^{j\to i}_R(x,y)\,\phi^j(x,y)\,dx\,dy = \sum_{\substack{j=1\\ j\neq i}}^{NG}\left(\Sigma^{j\to i}_{R2}\cdot v_2 + \Sigma^{j\to i}_{R3}\cdot v_3\right)\phi^j_{m,N}$$ (V-[illegible])

The source terms can be represented as a single term and as $S^i_{m,N}$, then

$$S^i_{m,N} = \left[\frac{\chi^i\nu}{\lambda}\sum_{j=1}^{NG}\left(\Sigma^j_{f2}\cdot v_2 + \Sigma^j_{f3}\cdot v_3\right) + \sum_{\substack{j=1\\ j\neq i}}^{NG}\left(\Sigma^{j\to i}_{R2}\cdot v_2 + \Sigma^{j\to i}_{R3}\cdot v_3\right)\right]\phi^j_{m,N}$$ (V-[illegible])

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

$$A^i_{m,n} = \Sigma_{t1} V_1 + \Sigma_{t3} V_3 - \left(B^i_{m,n} + C^i_{m,n} + D^i_{m,n} + E^i_{m,n} + \frac{Y^i_1 \Delta y_1 + Y^i_3 \Delta y_2}{2}\right)$$

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

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

$$D^i_{m,n} = -\frac{D^i_1 \Delta x_1}{2\Delta y_1}$$

$$E^i_{m,n} = -\frac{D^i_1 \Delta y_1 + D^i_3 \Delta y_2}{2\Delta x_1}$$

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

CHAPTER VI

SOLUTION OF THE FINITE DIFFERENCE EQUATIONS

We have now finished the discussion of the setting up of finite difference equations. The next problem is to solve these equations bearing in mind that a typical problem will have between 1000 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.

$$A = \begin{bmatrix}
a_{11} & b_{11} & & & & d_{11} & & & & & \\
c_{21} & a_{31} & b_{21} & & & & d_{21} & & & & \\
& c_{31} & a_{31} & b_{31} & & & & d_{31} & & & \\
& & \ddots & \ddots & \ddots & & & & \ddots & & \\
& & & c_{m1} & a_{m1} & b_{m1} & & & & \ddots & \\
c_{12} & & & & & c_{12} & a_{12} & b_{12} & & & \\
& c_{32} & & & & & c_{22} & a_{22} & b_{22} & & \\
& & \ddots & & & & & \ddots & \ddots & \ddots & \\
& & & \ddots & & & & & \ddots & \ddots & \ddots \\
& & & & & & & & & & a_{m2}
\end{bmatrix}$$

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

Let

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

where i is the group index.

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

$$A\,\emptyset = S \qquad \text{(VII-3)}$$

In matrix notation the elements of a column vector $\emptyset$ are denoted by $\emptyset_1$, $\emptyset_2$, ... and those of the coefficient matrix A by [illegible] Thus

$$\emptyset = \begin{bmatrix} \emptyset_1 \\ \emptyset_2 \\ \emptyset_3 \\ \vdots \\ \emptyset_{p-1} \\ \emptyset_p \end{bmatrix} \qquad A = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,p-1} & A_{1,p} \\ A_{2,1} & \cdots & \cdots & A_{2,p-1} & A_{2,p} \\ \vdots & & \ddots & & \vdots \\ A_{p-1,1} & \cdots & \cdots & \cdots & A_{p-1,p} \\ A_{p,1} & \cdots & \cdots & \cdots & A_{p,p} \end{bmatrix} \qquad \text{(VII-4)}$$

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

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

from which it is obvious that the dimension of the flux vector is P=M·N. 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 of A is equal to or greater than the sum of the absolute values of the off-diagonal elements of that row. Namely, the matrix A is diagonally dominant. The difference between the diagonal element and the magnitude of the off-diagonal sum is denoted by $h_{m,n}$ and is defined as

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

where $b_{m,n}$, $c_{m,n}$, $d_{m,n}$, and $e_{m,n}$ have been given in Chapter V. [illegible] condition $h_{m,n}$ is positive or zero. For mesh points adjacent to the boundary, the difference between diagonal and off-diagonal elements are still positive. For example, for the boundary mesh the difference is;

$$l^i_{m,n} + a^i_{m,n} - (b^i_{m,n} + c^i_{m,n} + e^i_{m,n}) \quad \text{--- (VI-6)}$$

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

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

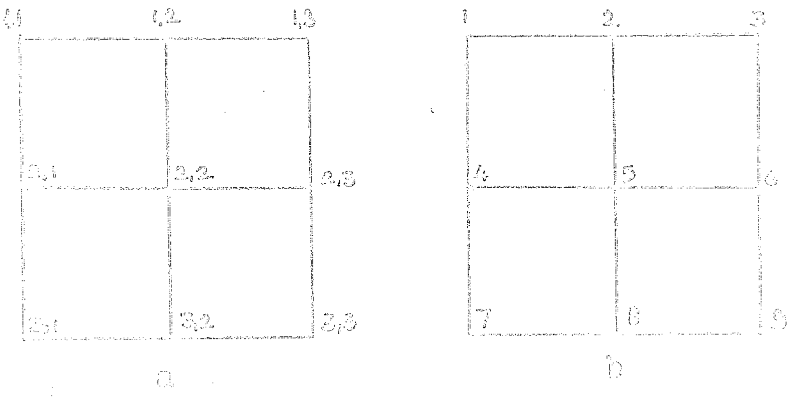


Figure VI-1

Notice that Equation (VI-7) is a pentadiagonal matrix. The mathematical properties of this matrix equation are [illegible]. We are particularly interested in the sufficient condition for the iterative solution to converge to the exact solution. The iterative solution is convergent if the spectral radius* of the iterative matrix is less than unity. Of course, it is generally very difficult or impossible to know all the eigenvalues of a matrix if the order of matrix is large. There are, however, theorems that give sufficient conditions to ensure a spectral radius less than unity. A proof of the theorems and a few of the basic propositions related to iterative convergence, can be found in textbooks on matrix theory, for example, Housholder (3) and Varga (4). In fact Equation (VI-3) has various favorable properties for iterative solution methods.

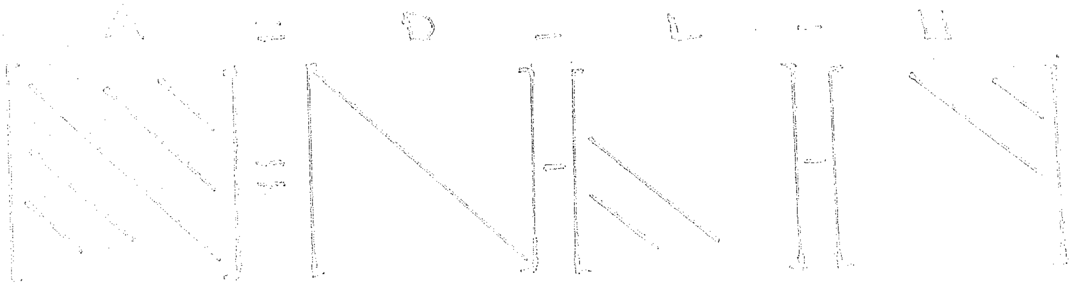
The following iterative schemes are well known
1. Point Jacobi iterative method.
2. Line Jacobi iterative method.
3. Gauss-Seidel iterative method.
4. Alternating direction implicit method.
5. Successive over relaxation method.
6. Cyclic Chebyshev semi iterative method.

VI-4 DETERMINATION OF THE ACCELERATION PARAMETERS FOR INNER ITERATION

We now return to the problem of solving Equation (VI-3). Let me illustrate the basic idea with a simple example. Suppose we wish to invert a matrix A, that is, we wish to solve

$$A\phi = S \qquad \text{(VI-5)}$$

The inner iteration procedure is set up to obtain an approximate solution of ϕ. Successive Over-relaxation method will be used for the inner iteration procedure. We first decompose A into the diagonal and off-diagonal elements.



(VI-6)

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*Spectral Radius of a matrix A is the number $\rho(A) = \max|\lambda|$, λ is an eigenvalue of A. It can be shown that $\|A\| \geq \rho(A)$, thus 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 iterative scheme even further by introducing an acceleration parameter to extrapolate the iterative flux estimate. This procedure is known as the Successive Overrelaxation (SOR) method. In the SOR method the displacement vector is w times 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. Of course for w=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 particularly important when the given problem is intrinsically slowly convergent. If the solution method employs the acceleration parameter repeatedly, it is worthwhile to develop a subprogram to calculate the optimal w. For this reason, subprogram VIN36 is provided.

Various methods of computing the accelerating parameter w has been investigated by B.A.Carre (5) who considered a problem for which the best value of w, denoted by w_{opt}, equals 1.9. This 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

$$\rho(G) = \rho^{2}(j) \qquad \text{(VI.[illegible])}$$

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

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 $\phi^{(1)}, \phi^{(2)} \ldots\ldots \phi^{(t)}$ to the solution of the P=M·N equations by Gauss-Seidel iterations and then estimates $\rho(G)$ from

$$\rho(G) = \lim_{t \to \infty} \frac{\| d^{(t+1)} \|}{\| d^{t} \|} \qquad \text{(VI.[illegible])}$$

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

$$\|d^{(t+1)}\| = |\phi^{(t+1)} - \phi^{t}| + |\phi^{(t+1)} - \phi^{t}| + \ldots + |\phi^{(t+1)} - \phi^{t}| \qquad \text{(VI.[illegible])}$$

or

$$\|d^{(t+1)}\| = \text{maximum of } |\phi_i^{(t+1)} - \phi_i^{(t)}| \qquad i=1,2,\ldots p \qquad \text{(VI.[illegible])}$$

$$\|n^{(t+1)}\| = \left[\left(\phi_1^{(t+1)} - \phi_1^{t}\right)^2 + \left(\phi_2^{(t+1)} - \phi_2^{(t)}\right)^2 + \dots + \left(\phi_p^{(t+1)} - \phi_p^{t}\right)^2\right]^{1/2} \qquad \text{(VI-18a)}$$

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

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

$$\mathrm{FOG}(\rho(G)) = \frac{2}{1+\sqrt{1-\rho(G)}} \qquad \text{(VI-19)}$$

If any one of the estimated values for ROMI, ROMA and RODE found by VIN-36 is greater than one, then VIN-36 makes a new estimate for them until they all are less than or equal to one. Then the program calculates maximum, minumum and average overrelaxation factors by using the function

$$\mathrm{FOG}(x) = \frac{2}{1+\sqrt{1-x}} \qquad \text{(VI-20)}$$

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

$$w_{max} = \frac{}{1+\sqrt{1-\rho_{max}(G)}} \qquad \text{(VI-21)}$$

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

$$w_{min} = \frac{2}{1+\sqrt{1-\rho_{min}(G)}} \qquad \text{(VI-22)}$$

$$w_{opt} = \frac{2}{1+\sqrt{1-\rho_{opt}(G)}} \qquad \text{(VI-23)}$$

after which ZT is obtained from

$$ZT = \frac{w_{max} - w_{min}}{2 - w_{opt}} \qquad \text{(VI-21)}$$

If ZT < 0.2 then calculation of the overrelaxation factors is completed and those 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 parameters to be found is determined and then as many of them are computed as follows;

$$w_1 = 1 \qquad \text{(VI-22)}$$

$$w_2 = \frac{2}{2 - \rho_{ave}(G)} \qquad \text{(VI-23)}$$

$$w_n = \frac{4}{4 - \rho_{ave}(G) \cdot w_{n-1}} \qquad \text{for } n > 2 \qquad \text{(VI-24)}$$

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

VI-8 STRATEGIES FOR SOLVING THE FINITE DIFFERENCED MULTIGROUP DIFFUSION EQUATIONS

If we recall the general discussion of finite difference formulations of the neutron diffusion equations given in Chapter V, it is apparent that the general structure of the finite differenced multigroup diffusion equations takes the form;

$$a^i_{m,n}\,\phi^i_{m,n} + b^i_{m,n}\,\phi^i_{m+1,n} + c^i_{m,n}\,\phi^i_{m-1,n} + d^i_{m,n}\,\phi^i_{m,n+1} + e^i_{m,n}\,\phi^i_{m,n-1} = S^i_{m,n} \qquad \text{(VI-25)}$$

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 P=M.N and the number of groups by NG, then Equation (VI-26) represents a set of P·NG simultaneous linear algebraic equations. One usually normalizes the flux at one energy group-space mesh point, since overall normalization of the flux is arbitrary in a criticality calculation. Hence, we have P·NG equations available to determine the (P-1).NG fluxes and the multiplication eigenvalue λ. As before, it is convenient to rewrite this set of equations as a matrix eigenvalue problem

$$A\phi = \frac{1}{\lambda} F\phi \tag{VI-27}$$

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 outer iterations which can be thought of as a ratio of the integral of neutron population at an 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

$$\psi = \frac{1}{\lambda} F\phi = \frac{1}{\lambda} S \tag{VI-28}$$

where

$$S = F\phi \tag{VI-29}$$

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

$$A\phi^{(t)} = \psi^{(t-1)} \qquad \text{(VI-32)}$$

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

$$S^{(t)} = F\phi^{(t)}. \qquad \text{(VI-33)}$$

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

$$\psi^{(t)} = \frac{1}{\lambda^{(t)}} S^{(t)} \qquad \text{(VI-34)}$$

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 $S^{(t)T}$ we obtain

$$\lambda^{(t)} = \frac{S^{(t)^T} . S^{(t)}}{S^{(t)^T} . \psi^{(t)}} \qquad \text{(VI-36)}$$

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

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

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

$$S^{(o)} = F\phi^{(o)} \qquad \text{(VI-37)}$$

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

$$\psi^{(o)} = \frac{1}{\lambda^{(o)}} S^{(o)} \qquad \text{(VI-38)}$$

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

$$A\phi^{(t)} = \frac{1}{\lambda^{(t-1)}} S^{(t-1)} \qquad \text{(VI-39)}$$

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 usually take the previous flux estimate $\phi_i^{(t-1)}$ as their first guess in solving Equation (VI-40). It should be mentioned that a variety 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 POINT FLUXES

VII-A SUBROUTINE NORMA

This routine evaluates the region average fluxes, performs 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 a part of input data by the total amount of energy production rate given 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 ERUDUS. As was explained in SERCON, this data, including microscopic cross sections, is first 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.

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

where

IG = group index

L = region index

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

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

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

$\Sigma_f(L,IG)$, being a part of macroscopic cross sections, will be computed in SERCON via the use of microscopic data and the self shielding factors. e (energy production per fission) is given as input. 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 performs an average burn-up, that is, assigns the same average isotopic number densities and macroscopic cross sections to a given region. Also each region consists of mesh grid. Each 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

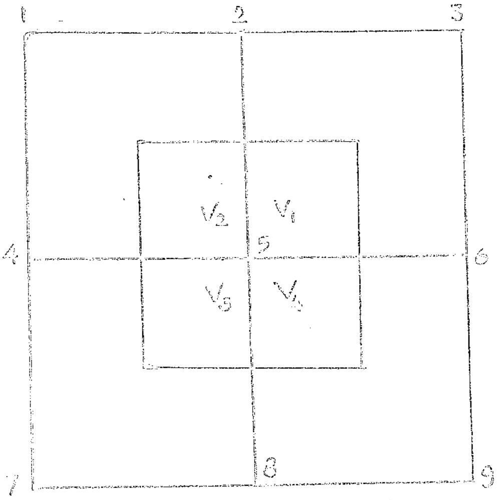


Figure VII-1

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 grid 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 firstly determines the neighbouring mesh points which are 4, 7, and 8. Each mesh point is known to belong to a specified region. After that, point fluxes for points 5, 4, 7 and 8 are evaluated and mesh volume elements around the point 5 are calculated by the following scheme.

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

$$XT1 = \Delta x . \Delta y \qquad \text{(VII-2)}$$

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

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

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

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

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, BCON(IG,1), is less than zero here then zero flux condition is obtained, in which case leakage from the top side of the reactor is

$$XLEK(IG,1)=D(L,IG)\cdot\frac{VET4(N3)+VET4(N4)-\left[VET4(N1)+VET4(N2)\right]}{\Delta y}\cdot\frac{\Delta x}{2}$$

(VII-5)

where

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

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

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

VII-6

At the left side of the reactor

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

(VII-7)

At the right side of the reactor

$$XLEK(IG,4)=D(L,IG)\cdot\frac{VET4(N1)+VET4(N3)-\left[VET4(N2)+VET\ 4(N4)\right]}{\Delta x}\cdot\frac{\Delta y}{2}$$

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

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

and total energy production in the whole reactor

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

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

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

where

XT is given as input and TOT is calculated.

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

Leakage from the reactor boundaries;

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

Actual neutron production $FNOR = \frac{1}{\lambda} FNOR.TOT \qquad (VII-13)$

Integrated actual power for region L;

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

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;

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

Integrated actual volume flux for region L and group IG;

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

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 here denoted by VOLTA;

$$\mathrm{VOLTA} = \sum_{\substack{L=1 \\ L \neq \mathrm{NEGL}}}^{\mathrm{NGREG}} \mathrm{VOL}(L) \qquad \text{(VII-18)}$$

where

NEGL : number of regions in which there is no energy generation

VOL(L) : volume of the region L

Actual power density

$$\mathrm{XY} = \frac{\mathrm{XASS}}{\mathrm{VOLTA}} \qquad \text{(VII-19)}$$

Average power density in region L; ZT1=ASS(L)/VOL(L)

Average source density for region L; ZT2=CFSOR(L)/VOL(L)

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

$$\mathrm{XYASS}(L) = \frac{\mathrm{ZT1}}{\mathrm{XY}} \qquad \text{(VII-20)}$$

VII-B SUBROUTINE OUTER

The goal of this subprogram is to determine the point [illegible] and fluxes. For this reason, OUTER calculates the loss and [illegible] contents in a reactor by making use of the group constants read in from logical unit number 4.

The loss terms include absorption, removal and leakage which are calculated separately in each region for the group IG. The absorption term is here denoted by ABSINT(IG)

$$\mathrm{ABSINT(IG)} = \sum_{L=1}^{NREG} \Sigma_a(L,IG).\phi(L,IG) \qquad \text{(VII-21)}$$

The removal term is

$$\mathrm{RMINT(IG)} = \sum_{L=1}^{NREG} \Sigma_r(L,IG).\phi(L,IG) \qquad \text{(VII-22)}$$

Transverse leakage

$$\mathrm{TRLEK(IG)} = \sum_{L=1}^{NREG} D(L,IG)B^2(L,IG).\phi(L,IG) \qquad \text{(VII-23)}$$

Leakage from the reactor boundaries have been obtained in HORMA. The source term includes sources due to fission and scattering collision.

Fission source

$$\mathrm{FSINT(IG)} = \frac{\nu}{\lambda} \sum_{L=1}^{NREG} \Sigma_f(L,IG).\phi(L,IG) \qquad \text{(VII-24)}$$

Scattering collision source or removal source:

$$\mathrm{SCSOR(IG)} = \sum_{L=1}^{NREG} \sum_{\substack{K=1 \\ K=IG}}^{IG} \Sigma_R(L,K).\phi(L,K) \qquad \text{(VII-25)}$$

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

$$OGA(IG) = \sum_{L=1}^{NREG} \nu \cdot e(IG) \Sigma_f (L,IG) \phi(L,IG) \qquad \text{(VII-26)}$$

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

$$ABSINT(IG) = ABSINT(IG) + RMINT(IG) + TRLEK(IG) \qquad \text{(VII-27)}$$

Total losses in the reactor denoted by XT2 is;

$$XT2 = \sum_{IG=1}^{NG} \left[ABSINT(IG) + \sum_{K=1}^{4} XLEK(IG,K) \right] \qquad \text{(VII-28)}$$

where

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

The sources in each group are given by;

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

$$\sum_{L=1}^{NREG} \sum_{\substack{K=1 \\ K \neq IG}}^{NG} \Sigma_R (L,K) \phi(L,K) \qquad \text{(VII-29)}$$

and the total source is determined as;

$$XT3 = \sum_{IG=1}^{NG} SCSOR(IG) \qquad \text{(VII-30)}$$

CHAPTER VIII

FUEL DEPLETION ANALYSIS

As energy production proceeds in the reactor, the fuel composition changes as a result of losses of fissionable material due to fission, build-up and decay of fission products, and transmutation of the reactor materials due to neutron capture. The analysis of core composition changes is complicated by the fact that the time and spatial variation in isotopic composition will depend on the neutron flux distribution which itself depends on the core composition. Fortunately changes in core composition occur relatively slowly (on time scales of hours, days or even months) so that the reactor core can be always be kept in a critical state by control element adjustments or by manipulating the soluble poison distribution. This means that although a time-dependent analysis of the rate equations describing the changes in isotopic number densities is necessary, the neutronic behavior can be studied by performing a sequence of instantaneous static criticality calculations for each core composition encountered at each time step of the burnup period.

Three aspects of depletion analysis are particularly important from the point of view of fuel management.

1. The reactivity loss rate associated with fuel depletion and its effect on the energy production during the cycle.

2. The changes in power distribution associated with depletion, including the effects of control poison adjustment to maintain criticality.

3. The change in fuel composition, with particular emphasis on those isotopes of greatest economic value so that the fuel cycle cost can be accurately evaluated.

The effects of depletion are evaluated by subdividing the time the fuel resides in the reactor into a sequence of time or burnup steps. A depletion analysis is then carried out for each [illegible] assuming separability in space and time. The [illegible] step in the evaluation is the calculation of a converged flux and/or power distribution for the spatial composition that exists at the beginning of the burnup step. This includes adjustment of control material to yield a critical or near critical eigenvalue. 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 assumed constant over the burnup time step. Finally, the energy production distribution is used to evaluate the changes in isotopic number densities during a depletion step. The process is then repeated for subsequent time steps until the reactor is almost subcritical with all control material removed, save that portion needed for daily operations, startup and shutdown.

During the depletion process, the neutron spectrum within the energy groups will also be subject to change. This change can be accounted for by recalculating the asymptotic neutron spectrum in each fuel type periodically during the depletion process and generating new fuel group constants for each depletion interval. This is equivalent to assuming separability of the neutron spectrum and time over the depletion time steps.

[illegible] THE BASIC EQUATIONS OF ISOTOPIC TRANSMUTATION 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:

$$\frac{dN^j}{dt} = -N^j\Big[\lambda^j + \sum_{i=1}^{NG} \sigma_a^{i,j} f^{i,j} \phi^i(x)\Big] + \lambda^{PD} N^{PD} + N^{PC} \sum_{i=1}^{NG} \sigma_c^{i,PC} f^{i,PC} \phi^i(x)$$

$$+ N^{P2} \sum_{i=1}^{NG} \sigma_c^{i,P2} f^{i,P2} \phi^i(x) + \sum_{l=1}^{NFS} y^{l\to PD} N^l \sum_{i=1}^{NG} \sigma_f^{i,l} f^{i,l} \phi^i(x) \quad [illegible]$$

with:

NG: number of groups

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

$\phi^i(x)$: average flux over the considered region and group i

λ^j: decay constant of isotope j

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

M1,M2,M3 : indices of the capture parents 1 and 2 and decay parent respectively

The time rate of change of the concentration of isotope j in equation (VIII-1) is based on two loss modes and three production modes. The two modes, by which the nuclei of isotope j are lost, are :

1. The first term represents the loss by radioactive decay of isotope j with decay constant λ^{j}.
2. The second term represents loss by neutron absorption with a spectrum averaged microscopic cross section σ^{j} including fission and capture.
3. The third term in Equation VIII-1 represents production by radioactive decay of precursor, N^{m3}, with a decay constant, λ^{m3}. Production of a given isotope can be by more than one type of decay. As an example, X^{135} can be generated by beta decay of I^{135}.
4. The fourth term represents production by neutron interaction with a precursor species N^{m1} by neutron capture with σ^{m1}. As an example, U^{237} is produced as a result of an (n,γ) reaction in U^{236}.
5. The fifth term represents production by precursor species N^{m2} by neutron capture with cross section σ^{m2}.
6. The final term in Equation VIII-1 represents the production term for fission products, where the value of the fission product yield, γ^{j}, is dependent on both the fissioning isotope and the energy of the neutron causing fission.

Note that Equation (VIII-1) is nonlinear if either the flux or the reaction cross sections are time dependent. In [illegible] the time or burn-up step length can be chosen [illegible] the neutron spectrum, and hence the cross sections, [illegible] do [illegible] variation. Assuming a constant flux over the [illegible] however, is a more severe restriction. [illegible] however, Equation (VIII-1) will be linear. [illegible] cases, linearization can be accomplished by restricting the range of other operating variables. Our objective in beginning with the general equation is to emphasize that simplification of the differential equations for transmutation and decay is usually obtained at the expense of placing restrictions on the 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 burnup cycle by creation of new fissile material. The two most common fertile nuclides are Th^{232} and U^{238}. The production chains for these isotopes are shown in Figure VIII-1 and VIII-2. If the captures in fertile nuclei exceeds the absorption in fissile ma-

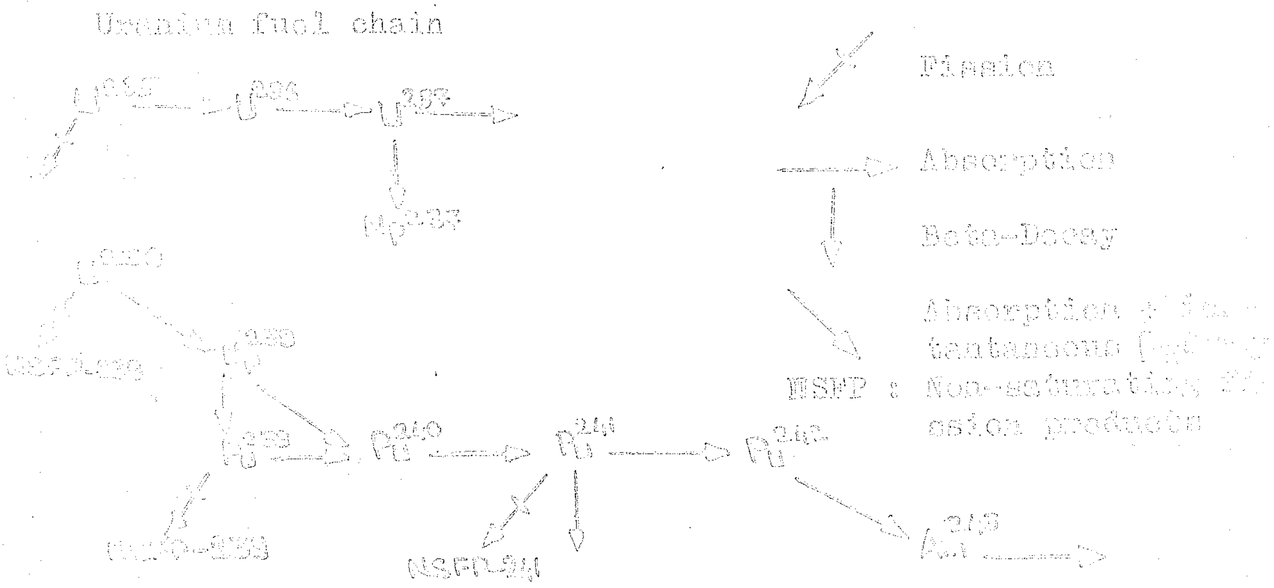


Figure VIII-1 Isotopic chains of interest in fuel depletion analysis.

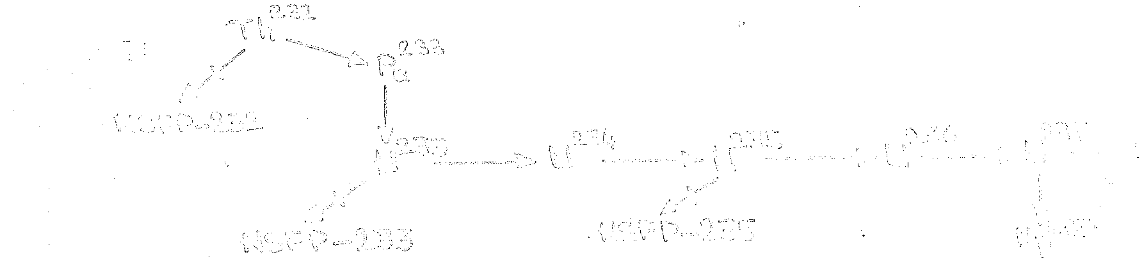


Figure VIII-2 Isotopic chains of interest in fuel depletion analysis.

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 instantoneous 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 largest 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 supercript. The first digit in the supercript is the last digit ofthe atomic number of the nucleus, and the second digit is the last digit of the mass number. The U^{238} concentration is then represented by N^{28}, and Pu^{239} by N^{49}. The differential equations describing the chain in Figure VIII-1 are then;

$$\frac{dN^{28}}{dt} = -\sigma_a^{28} N^{28} \phi \qquad \text{(VIII-2)}$$

$$\frac{dN^{29}}{dt} = \sigma_c^{28} N^{28} \phi - \lambda^{29} N^{29} \qquad \text{(VIII-3)}$$

$$\frac{dN^{39}}{dt} = \lambda^{29} N^{29} - \lambda^{39} N^{39} \qquad \text{(VIII-4)}$$

$$\frac{dN^{49}}{dt} = \lambda^{39} N^{39} - \sigma_a^{49} N^{49} \phi \qquad \text{(VIII-5)}$$

$$\frac{dN^{40}}{dt} = \sigma_c^{49} N^{49} \phi - N^{40} \sigma_a^{40} \phi \qquad \text{(VIII-6)}$$

$$\frac{dN^{41}}{dt} = \sigma_c^{40} N^{40} \phi - N^{41} (\lambda^{41} + \sigma_a^{41} \phi) \qquad \text{(VIII-7)}$$

$$\frac{dN^{42}}{dt} = \sigma_c^{41} N^{41} \phi - \sigma_a^{42} N^{42} \phi \qquad \text{(VIII-8)}$$

In Equations (VIII-2) to (VIII-8), 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 losses by radioactive decay. We can obtain considerable additional simplification if we assume that the time span of interest is long compared to the inverse decay constants of U^{239} and Np^{239}. The effect 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}

$$\frac{dN^{49}}{dt} = \sigma_c^{28} N^{28} \phi - \sigma_a^{49} N^{49} \phi \qquad \text{(VIII-9)}$$

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

$$\Theta = \int_0^{\tau} \phi(t)\, dt \qquad \text{(VIII-10)}$$

we have the following coupled set of linear equations:

$$\frac{dN^{28}}{d\Theta} = -\sigma_a^{28} N^{28} \qquad \text{(VIII-11)}$$

$$\frac{dN^{49}}{d\Theta} = \sigma_c^{28} N^{28} - \sigma_a^{49} N^{49} \qquad \text{(VIII-12)}$$

$$\frac{dN^{40}}{d\Theta} = -\sigma_a^{40} N^{40} + \sigma_c^{49} N^{49} \qquad \text{(VIII-13)}$$

$$\frac{dN^{41}}{d\Theta} = \sigma_c^{40} N^{40} - \sigma_a^{41} N^{41} - \frac{\lambda^{41} N^{41}}{\phi} \qquad \text{(VIII-14)}$$

$$\frac{dN^{42}}{d\Theta} = \sigma_c^{41} N^{41} - \sigma_a^{42} N^{42} \qquad \text{(VIII-15)}$$

The last term in Equation VIII-14 is normally neglected in evaluating fuel composition changes within the reactor. Although this causes an error of less than 1% during reactor operation, radioactive decay of Pu^{241} (half life=15 years) is appreciable over the time periods between discharge from the reactor and fuel reprocessing. For high burnup fuels, or fuels initially loaded with a mixture of fissile Plutonium isotopes, it is sometimes necessary to account for the neutron poisoning effects of other transplutonium 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 of the 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^i is the spectrum averaged microscopic cross section for absorption in isotope N^i and σ_c^i is the spectrum averaged microscopic cross section for capture to produce the next higher isotope in the chain from isotope N^i. If more than one isotope of the chain is present at the beginning of a fuel burnup step, the same series of equations can be used to determine the contribution of each initial isotope to the total concentration of any 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 if two of the one group microscopic absorption cross sections are close to one another 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;

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

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

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

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

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

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

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

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

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

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

VIII-B FISSION PRODUCT POISONING

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

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

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

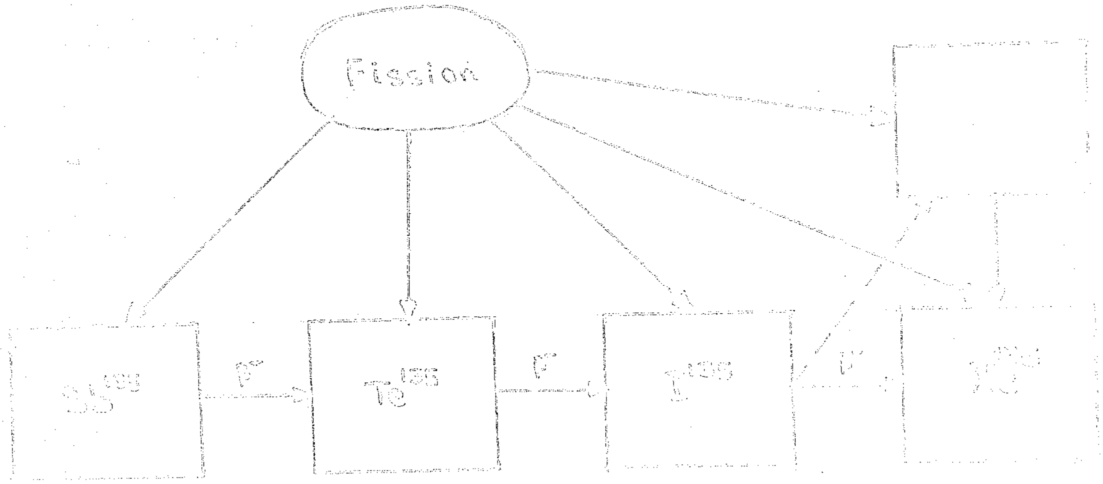


Figure VIII-3 A portion of the decay scheme for A=135.

Fortunately this rather complicated decay scheme can be considerably simplified by assuming that the decay of Te^{135} to I^{135} is instantaneous. Furthermore we will also ignore the short lived 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 isotopes as $N^I(t)$ and $N^X(t)$ respectively. Furthermore let γ_I and γ_X denote 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 coupled rate equations describing the simplified decay scheme illustrated in Figure VIII-4

Iodine

$$\frac{\partial N^I}{\partial t} = \gamma_I \Sigma_f \phi - \lambda_I N^I \qquad \text{(VIII-24)}$$

Xenon

$$\frac{\partial N^X}{\partial t} = \gamma_X \Sigma_f \phi + \lambda_I N^I - \lambda_X N^X - N^X \sigma_a^X \phi \qquad \text{(VIII-25)}$$

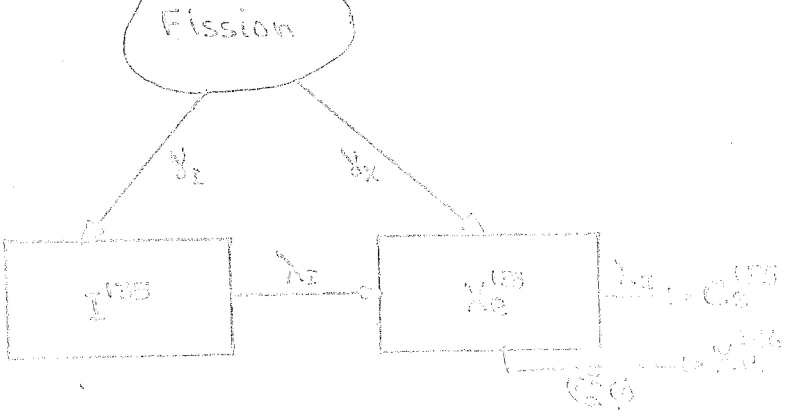


Figure VIII-4 A simplified decay scheme for Xe^{135}

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

$$N^I(t)=\frac{\gamma_I\Sigma_f\phi}{\lambda_I}\left(1-e^{-\lambda_I t}\right) \qquad \text{(VIII-26)}$$

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

$$N^X(t)=\frac{(\gamma_I+\gamma_X)\Sigma_f\phi}{\lambda_X+\sigma_a^X\phi}\left[1-e^{-(\lambda_X+\sigma_a^X\phi)t}\right]+\frac{\gamma_I\Sigma_f\phi}{\lambda_X-\lambda_I+\sigma_a^X\phi}\left[e^{-(\lambda_X+\sigma_a^X\phi)t}-e^{-\lambda_I t}\right] \qquad \text{(VIII-27)}$$

That is, the concentration of these fission product poisons in a reactor operating at constant flux will eventually saturate at those equilibrium values for which the production of poisons from fission is just balanced by the decay and neutron capture losses of the poisons. These equilibrium concentrations could also have been determined directly from the rate equations VIII-24 and 25 themselves by merely setting $dN^I/dt = 0 = dN^X/dt$

VIII-6 SUBROUTINES DEPL , SHIED , DBURN , [illegible] , BBB and SUBDEP

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

Subroutine DEPL is used to calculate the normalization factor and the normalized flux. For the calculation of the normalization factor it is necessary to have self shielding factors and the group constants. Self shielding factors are calculated by the subprogram SHIED. The method of calculating the self shielding factors is the same as that described in the subprogram SEIGGI. Also the same procedure, explained in NORMA, is followed to calculate the normalization factor and the normalized fluxes.

After calculating the normalized flux, burnup calculations for a small time step starts. For this reason, the loss and source terms of the depletion equation are calculated separately.

There are two loss termsos explained before. Absorption is denoted by WABS(J) ;

$$WABS(J) = \sum_{IG=1}^{NG} \sigma_a(IG,J)\, \xi(IG,J)\, \phi(L,IG) \qquad \text{(VIII-28)}$$

the radioactive decay is denoted by DEC(J);

$$DEC(J) = \lambda(J) \qquad \text{(VIII-29)}$$

There are foue source terms which are also as explained before. Fission is donoted by;

$$WFIS(J) = \sum_{IG=1}^{NG} \sigma_f(IG,J)\, \xi(IG,J)\, \phi(L,IG) \qquad \text{(VIII-30)}$$

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

$$WCAP(J) = WABS(J) - WFIS(J) \qquad \text{(VIII-31)}$$

Gain due to beta decay;

$$BBETA(J) = DEC(J) \qquad \text{(VIII-32)}$$

Fission yield is;

$$YIELD(J,I) = GAM(J,I,NI) \quad (VIII-33)$$

Decay constants and fission yields have been given as input.

After that, subprogram DEPL calls subprogram DBURN for constituting the depletion matrix which is called DEPM. It is lower triangular matrix. Diagonal elements of DEPM is constituted by:

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

The other elements of the depletion matrix are placed in DEPM. DEPL calls subprogram SPLIT which splits the given depletion matrix DEPM into NFLCHN independent of fuel and (NCHAIN-NFLCHN) fission product chains. Each chain is characterized by the parameters NSPLIT(L) which is the index of the first member of chain L.

NORA(K), (K=1,2 ... NCHAIN) is the width of the stripped matrix. After [illegible] splitting the depletion matrix, subprogram [illegible] and [illegible] solve each depletion submatrix equation separately by using an analytical approach.

CHAPTER IX

DISCUSSION AND SUGGESTIONS FOR FURTHER WORK

This study was to form the second part of a larger problem concerning the possibility of power production alongside with U^{233} conversion from Th^{232} in a conventional PWR of the [illegible] offered for the AKKUYU plant. The first part has made use of the PWR spectral code GELS developed by K. Ponndorf, F. Schult, [illegible] Bohm under the auspices of GKSS (Gesellschaft für Kernenergieverwertung in Schiffbau und Schiffahrt mbH.) to generate broad group constants for reactor cells made up of varying mixtures of [illegible] fuel elements in which the Uranium component is enriched to different levels between 12%and 20% $U^{235}$by weight. Similar computations for supercells containing lumped control poison was generated by that study (21)

In this work the intention was to study the multigroup diffusion depletion program "EREBUS" in two dimensions with a [illegible] of approach so as the prepare an enlarged manual for possible users and adapt the code to the UNIVAC-1106 system at Hacettepe University. This has been accomplished to a large extent but successful trial runs proved to be not possible due to the difficulties encountered in attempts to have access to the data [illegible] that was supposed to be generated by the GELS code for EREBUS. The possibility of using the card input medium to run the code was precluded because of the tremendous volume of input data required by EREBUS. Thus the study remained confined to a theoretical outline of the code and debugging of compilation errors in adaptation to UNIVAC-1106system.

Further work along these lines could involve first of all removing the obstacle to successful utilization of the [illegible] by EREBUS and then using the code to analyze reactor configurations composed of different cell regions for which the necessary data would be generated by GELS. There is clearly [illegible] approach to the design of a PWR that would be [illegible] U^{233} without sacrificing from the other desirable performance [illegible]teristics. For example, placing a Thorium rich fuel near the center of the core would result in high conversion but power [illegible] would be adversely affected at least for a few initial [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_{eff} values and thus sufficiently long core lifetime. On the other hand, an inclination to place the Thorium rich cell more at the periphery of the core would be good for neutron economy since Thorium conversion is more effectively done with low energy neutrons and also because the neutrons in peripheral regions would be lost through leakage from the system anyway. Thus the core designer would have to try different core configurations while being guided by considerations of this kind and choose the design that performs best according to the criteria of Thorium conversion, power production, uniformity of power 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 programmers on the IBM-360 is not yet definitely settled, and is likely to undergo changes in the near future. Therefore, in view of possible future restrictions on the machine available storage, the limitations of EREBUS can not be specified on this study, so they are indicated parametrically. The numerical values of these parameters, for the present version of EREBUS now running at Ispra, are given in appendix B, so that future changes of the program restrictions will only imply the updating of appendix B.

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

The input data have been divided into 13 card sets (each set may contain one or more cards):

1.: TITLE CARD (18A4)

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

2.: CARD No. 2 (24I3)

Col. 1-3 NG ($\leq$KGD) = number of groups.
Col. 4-6 NREG ($\leq$ KREG) = number of regions.
Col. 7-9 NCMP ($\leq$ KCD) = number of composition
Col. 10-12 NIS ($\leq$ KIS) = maximum isotope index.
Col. 13-15 NPY ($\leq$ KYD) = number of rows.
Col. 16-18 NPX ($\leq$ KXD) = number of columns.
N.B.: It must be NPX·NPY $\leq$ KPD or, for a symmetric case (NPX+1)·NPX/2 $\leq$ KPD ([illegible]).
Col. 19-21 NT = maximum number of outer iterations.

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 case)

Col. 25-27 IDG = 1 the initial flux approximation, for the time step zero; is read from tape.
= 0 is read from cards, per group.
=-1 is read from cards, per composition and per group.
=-2 is read from cards, per region and per 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 Gauss-Seidel matrices, in the first criticality 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 removal matrix is not printed

Col. 40-42 IMACR1= If this field is zero or blank, the [illegible] shielding factor is not printed.

Col. 43-45 IPRINT= print index. If IPRINT = 1, then the program prints the selective information.

3.3 CARD No. 3 (24I3)

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

Col. 4-6 NRUN = last time step to be completed in the present run (NRUN $\leq$ NGRINT)
If NRUN=NGRINT, the program ends after

the diffusion calculations of the time-step NGRINT.
If NRUN≤NGRINT, the program ends after the computation of the number densities and the saving of data for restart, and before the fuel shuffling and the diffusion calculations of the time step NRUN+1.

Col. 7-9 NGEOM = 0 x, y geometry.
= 1 r, z geometry.
Col. 10-12 IDIAG = 1 the reactor is symmetric about the 45° main diagonal. In this case it must be:
NPX=NPY and NPX·(NPX+1)/2≤KPD.
= 0 no diagonal symmetry.
Col. 13-15 ICOND = 0 the boundary conditions are the same for all groups.
= 1 the boundary conditions are group dependent.
Col. 16-18 IPOW = 0 only one power all through the lifetime.
= 1 the power is specified for each time step.
= 2 the power is specified for each sub time-step.
If NGRINT=0, it must be IPOW=0.
Col. 19-21 IBK = 0 one buckling.
= 1 buckling per group.
= 2 buckling per group and per [illegible]
= 3 buckling per group and per [illegible]
Col. 22-24 ISYST = 0 the microscopic cross sections are given in barns, and the number [illegible] in Szilard (1 Szilard=10^{24} [illegible]
= 1 the cross section are given in [illegible] the number densities in [illegible]
Col. 25-27 NSFZ = 0 the self shielding factors are [illegible]ated by formula (IV-24).
= 1 the self shielding factors are [illegible]ated by the polynomial formula [illegible]
Col. 28-30 ICRISE = 0 straight burnup.
= 1 search of the dilution factor [illegible]
= 2 regionwise programmed search of [illegible]trol isotope number density.
= 3 boundary search.

Col. 31-33 NCRIT = maximum number of criticality iterations. Note that, in the boundary searches, one criticality iteration means a boundary displacement of one "elementary step" (thus one mesh row).

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

Col. 37-39 NIF = number of fuel isotopes. All isotopes are from 1 to NIF are considered fissionable. It must be NIF ≤ NUCL. (NIF ≤ KIF)

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

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

4 : SPECIFICATION FOR THE GROUP-FLUX PRINTING

This set of one or more cards (24I3), present only if [illegible] is equal to one, on card no.2, specifies the vector IP(I) I=1,2,.....NG

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

Col. 4-6 IP(2) = the same meaning for the group 2, and so on for all groups. If NG>24, two or more cards are needed.

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

Col. 1-10 AUTCRI = eigenvalue λ_c to be searched for, in the criticality searches (ICRISE = 1,2,3)
= minimum allowed eigenvalue λ_{min}, if ICRISE= 0. If the multiplication factor, at some time step, becomes less than λ_{min} the calculation is stopped. If this field contains zero or is left blank, the program assumes AUTCRI = 1 .

Col. 11-20 AUT = initial eigenvalue approximation. If this field is zero or blank, the program assumes AUT = 1 . This value is used only if ILAM = 0 on CARD No.2 .

Col. 21-30 SIGMA = initial guess of the dominance ratio (= ratio between the second and the first eigenvalue λ, if the eigenvalue are [illegible] dered by decreasing modulus). It must be $\zeta<1$. If this field is left blank or contain zero, and ISIG=0 on card no.2, ζ is calculated by the program.

Col. 31-40 ETA = convergence criterion for the criticality searches (ICRISE = 0). This search is interrupted when $|\lambda-\lambda_c|<$ ETA

Col. 41-50 EPS = pointwise convergence criterion :

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

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

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

Col. 61-63 DEL = Convergence criterion for inner iterations. If this field is zero or left blank, the program sets automatically DEL=0.1 .

Col. 64-66 TAU = Convergence criterion for overrelaxation factor. If this field is zero or left blank, the program sets automatically TAU=0.2 .

6 : CARD No. 6 SPECTRAL RADII OF GAUSS-SEIDEL MATRIX

This set consists of one or more cards (7E10.5) if NOM = 1.

Col. 1-10 OGA(1)= spectral radius of Gauss-Seidel matrix for group 1

Col. 11-20 OGA(2)= same for group 2.

And so forth, up to OGA(NG).

7 : BOUNDARY CONDITIONS

KIKEUF applies on each external side of the reactor, condition of type :

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

where $\alpha^i \geq 0$, $\beta^i \geq 0$, $\alpha^i+\beta^i > 0$.

This set consists of one card (8E9.4) if ICOND = 0 or NG cards if ICOND = 1 .

$$\left.\begin{array}{ll}\text{Col. 1-9} & \alpha^i\\ \text{10-18} & \beta^i\end{array}\right\}\text{ for the top side (row 1)}$$

$$\left.\begin{array}{ll}\text{Col. 19-27} & \alpha^i\\ \text{28-36} & \beta^i\end{array}\right\}\text{ for the left side (column 1)}$$

$$\left.\begin{array}{ll}\text{Col. 37-45} & \alpha^i\\ \text{46-54} & \beta^i\end{array}\right\}\text{ for the bottom side (row NPY)}$$

$$\left.\begin{array}{ll}\text{Col. 55-63} & \alpha^i\\ \text{64-72} & \beta^i\end{array}\right\}\text{ for the right side (column NPX)}$$

8 : SHUFFLING TIME-STEPS

This set of one or more cards (24I3), present only if NGRINT is greater than zero, is to specify the vector NFU(K), K are numbered, starting from one to NGRINT.
If NFU(K) = 1, the program performs the shuffling before the diffusion calculation of the time-step K. If NFU(K) = 0 no shuffling is performed. It is not possible to perform any shuffling at time-step zero.

9 : SMALL TIME-STEP DIVISION

This set of one or more cards (24I3), present only if NGRINT 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 the time-step 1 is divided.

Col. 4-6 NSA(2) = number of small time-steps, into which the 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 (8E10.5) :

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 stop 2
and so forth, up to W(NGRINT).

At any time stop K, the fluxos are normalized in such a way that :

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

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 FINDAC. The card sets below are read by the subprograms SINDAC and DEIR

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 column up to which this value is extended. All the C must be given in an increasing order, and the last one must be NPX.

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 NPY.
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 ($1 \leqslant c_1 \leqslant$NPX)

Col. 7-9 c_2= right column bounding the block ($1 \leqslant c_1 < c_2 \leqslant$NPX)

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

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

Col. 16-18 = Generally those columns are to be left blank Only when ICRISE=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 NUCL>0 (Card no.3). there must be NUCL cards (2A4, 3I4, 2E10.5), one for each time dependent isotope, folowing order of the isotope index from one to NUCL.

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

Col. 9-12 No_1= index of the first capture parent

Col. 13-16 No_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 Nc_1, Nc_2, N_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 NREG 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 NREG bucklings.

21 : INFORMATION CARD

There must be one card (24I3) containing :

Col. 1-3 NEC = number of isotopes whose number densitie are given per composition ($0 \leq NEC \leq NIS$).

Col. 4-6 NEMIR = number of isotopes whose number densitie are given per region ($0 \leq NEMIR \leq NUCL+1$).

Col. 7-9 NRC = number of compositions having logarithmi derivatives ($0 \leq NRC \leq NCMP$)

Col. 10-12 IPUN = 1, the number densities of the first NUCL+1 isotopes are punched on cards (7E10.5) at each time step, before the shuffling.

IPUN = 0, no punch cards.

These punched cards can be used to input the number densitie per region in other problems.

22 : NUMBER DENSITIES PER COMPOSITION

This set of cards, present only if NEC $\neq$ 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 NCMP number densities, one per composition.

Initialize a new card when changing isotope.

23 : NUMBER DENSITIES PER REGION

This set of cards, present only if NEMTR $\neq 0$, 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 NRC $\neq 0$ is constituted of :

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

24.b) NRC sets of cards (7E10.5), one for each composition, containing the logarithmic derivative C_i , i=1,2,.....,NG.

Initialize a new card, when changing the composition.

If $C_i > 0$, the composition under consideration is a "rod material" with respect to the group i; in this case the flux ϕ^i is not evaluated in the mesh points inside the composition, but it must satisfy, on the boundary points, the condition is

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

If $C_i = 0$, 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,....NG) for all groups.

It must be $\chi^i \geq 0$ and $\sum_{i=1}^{NG} \chi^i > 0$.

SINDAC
DELR

26 : DATA FOR THE UNIFORM SEARCH

Only if ICRIST = 1, there must be one card (7E10.5) containing :

Col. 1-10 DILMIN = Θ_{min} = minimum permissible value of th dilution factor .

Col. 11-20 DILMAX = Θ_{max} = maximum permissible value of th dilution factor .

27 : CONTROL LIST FOR THE REGIONWISE PROGRAMMED SEARCH

This set, present only when ICRISE = 2 , specifies the control list. It is made of as many cards (18I3, 2E9.4) 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 ($N_{min} < N_{max}$).

These number densities are given in Szilard or in nuclei/cm according to the option ISYST in card no.3 .

The same region can be repeated in two or more different banks. The maximum number of control bank is KLIST, and the total number of all region indices appearing in this set must not be greater than KTRL.

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 th regions belonging to the control list.

28 : BLANK CARD (only if ICRISE = 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 ICRISE=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 ($y_{min} < y_{max}$)

The same control area can be repeated in two or more different banks. The maximum number of control banks is KLIST. The entries of the control list (i.e. all the area indices appearing in the cards above) must not be more than KTRL. 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.

TINDAC

31 : LIBRARY AND SELF SHIELDING PARAMETERS
It is possible, in EREBUS, 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 compositio
a well determined LIBRARY SET and a SELF-SHIELDING SET.
The following card (24I3) provides general informations :

Col. 1-3 NBL=INX1= total number of library sets ($NBL \leq KBL$)
If $NBL > 0$, NBL sets of microscopic cross sectio
must be supplied consecutively, by means of as many data sets in NCELS file "SPECIFICATION OF ON
LIBRARY SET"
If NBL = 0, possible only if a WEAK RESTART case is dealt with, the program takes library data fro
the RESTART TAPE .

Col. 4-6 NBS=INX2= total number of self-shielding sets ($NBS \leq KBS$)
If $NBS > 0$, NBS sets of self-shielding coefficien
must be supplied consecutively by means of as man
card sets 33: SPECIFICATION OF ONE SELF-SHIELDING SET, ending with the card 34: SELF-SHIELDING ASSIGNEMENT which assigns the various self-shielding sets to the compositions.
If NBS=0, no self-shielding data (neither SELF-SHIELDING SPECIFICATION nor SELF-SHIELDING ASSIGNEMENT) are supplied on cards but the program reads them from the RESTART TAPE if the case und

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 n_c+1 (NGP $\geq$ 7)

SPECIFICATIONOF ONE LIBRARY SET

The description of this data set applies to one generic library set. If library set number (NBL) is greater than one, NBL such setsof 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 of the nonburnable isotopes.

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

c.) IDEP = 0, This isotope is included in the summation (CHAT-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 dens 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 other sets.

d.) If this alphameric field is not blank (e.g. contains the 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 last isotope of the set.

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

g.) The microscopic absorption cross sections σ^i_a (i=1,2,...NG).

h.) The microscopic removal cross sections σ^i_R (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 NIF, data i.), k.), l.), m.) must be supplied, otherwise they are omitted.

i.) The microscopic fission cross sections σ^i_f (i=1,2,....NG)

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

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

m.) The fission yields $\sigma^{k\to j}_{kR}$ (j=NIF+1, NIF+2,.....,NIF+NIP) of the isotope under consideration (k) for all fission products.

n.) This set is present only if the stage d.) has the word SCATTER. It is one of NG sets containing the microscopic removal cross sections $\sigma^{i\to j}_R$ (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 assignment 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 SELF-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 (NBS > 1) NBS 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·NCP coefficients (for all groups).

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

coefficients of the set K under consideration. It must be NBT(K) $\neq 0$.

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 NGP. .

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 :

$$NG \cdot NGP \sum_{K=1}^{NBS} NBT(K) \leqslant KCOF$$

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 SET 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
ting 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.

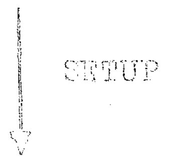
Col. 7-9 L(2) = second element of the list.

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 desities 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 EREBUS 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	IQERL = 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 subject 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 information~~s~~ concerning the use of peripheral units).

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