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RBU
CALCULATION OF REACTOR HISTORY INCLUDING
THE DETAILS OF ISOTOPIC CONCENTRATION
PART I: THE METHOD

By

E. J. Leshan
J. R. Burr R. Morrison
M. Temme G. T. Thompson

American-Standard

and

J. R. Triplett
Hanford Laboratories Operation

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Approved By:

J. W. Webster, Head
Reactor Physics Section

C. M. Rice, Manager
Reactor Engineering Department

A M E R I C A N - S T A N D A R D
Atomic Energy Division - Mountain View, California

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ABSTRACT

RBU is a digital computer program for the detailed calculation of the neutron, reactivity, and isotopic history of a reactor in which relatively exact models of the geometry and physical processes are included to permit reliable predictions of fuel costs and reactor performance. The program uses the monte carlo method to obtain the fine structure of the neutron flux in three space dimensions and energy. Using this fine structure, cross sections are averaged over space and energy to obtain the neutronic properties for **equivalent** homogeneous one-dimensional regions of space and ranges of energy. These are used in diffusion calculations to obtain the macroscopic flux distribution throughout the reactor. The consumption and production of isotopes is computed for a time step by the solution of sets of partial differential equations involving both the macroscopic and microscopic fluxes. With the new concentrations, diffusion calculations are performed again to obtain macroscopic fluxes for the next time step. At variable intervals monte carlo calculations are again performed to determine the changes in microscopic flux distributions. The cycle is repeated until conditions on the reactivity or other properties dictate the end of the calculation.

Programmed control rod manipulation or fuel transfers may be included in the calculation.

The monte carlo, diffusion, or burnup portions of the program may be used separately, on the IBM 704 as well as on the IBM 709 for which the complete program is written.

The unresolved resonance range is treated by random selection of resonance parameters from appropriate distributions using the Doppler broadened single level Breit-Wigner formula. Resolved resonances are treated similarly with the exception that specific values of the resonance parameters are used. The effects of molecular binding and thermal motion of the nuclei on near-thermal scattering are treated by a simple model capable of incorporating the pertinent physical theory and data.

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I. INTRODUCTION

The purpose of this report is to describe a method of predicting the reactivity and the distribution of isotopes in a nuclear power reactor as functions of its operating history.

The problem has, of course, been frequently approached using approximations of varying complexity, the accuracy and applicability of which are to some extent uncertain. In the method presented in this report, an attempt is made to eliminate most of the uncertain approximations in order to increase the range of applicability of the calculations. A digital computer program, RBU, using this method is being developed for the IBM 709 by the American-Standard Atomic Energy Division under contract with the Hanford Laboratories.

In this report a statement of the problem will be given, first; second, the concepts of microscopic and macroscopic flux are mathematically described; third, the method of approach is outlined; fourth, various sections are presented which describe the monte carlo portion of the code, the diffusion calculation, the burnup calculation, and the preparation of the various constants and cross sections needed in the program.

II. STATEMENT OF THE PROBLEM

Essentially the problem is one of determining the spatial and energy distribution of the neutron flux; the reactivity at a given time may be computed from the integrals over volume and energy of the products of various nuclear constants with the flux and from the integral over the outer surface of the reactor of the normal component of the flux. Similarly, the rate at which the various isotopes are consumed and produced at each point in the reactor may be computed from the integral over energy of the product of neutron flux and the cross sections for the relevant processes and from the decay constants for those nuclides which are radioactive. The determination of the neutron flux is complicated by the rapid variation of some cross sections with energy and of some concentrations with position in the reactor. Because of this extreme fluctuation, a very fine coordinate spacing is required for a reliable solution until sufficient experience has been acquired to permit generally valid approximations to be made. For this reason and because of the complex geometry involved in some fuel elements and control systems of interest, the monte carlo method is used in RBU for some of the neutron flux calculations. The program then uses the monte carlo results to obtain constants with which most of the flux determinations can be made by simpler methods.

III. MICROSCOPIC AND MACROSCOPIC FLUXES

In the following section the theoretical basis for the process of averaging over heterogeneities and of forming a one-space dimensional model for a three dimensional system is briefly discussed.

The neutron transport equation

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi(\vec{r}, \vec{v})}{\partial t} = & - \frac{1}{v} \vec{v} \cdot \vec{\nabla} \phi(\vec{r}, \vec{v}) - \Sigma_t(\vec{r}, v) \phi(\vec{r}, \vec{v}) \\ & + \int d\vec{v}' \left[\frac{1}{4\pi} v_f(\vec{r}, v') \Sigma_f(\vec{r}, v') \chi_f(v) \right. \\ & \left. + \frac{1}{4\pi} v_{in}(\vec{r}, v') \Sigma_{in}(\vec{r}, v' \rightarrow v) + \Sigma_s(\vec{r}, \vec{v}' \rightarrow \vec{v}) \right] \phi(\vec{r}, \vec{v}') \quad (1) \end{aligned}$$

expresses the rate at which the density of neutrons increases at each point in phase space in terms of the neutron flux density, its gradient and the various nuclear cross sections. If the region between $(\vec{r}, v, \vec{\Omega})$ and $(\vec{r} + \Delta\vec{r}, v + \Delta v, \vec{\Omega})$ is denoted as cell i , Equation (1) may be integrated over the cell as follows:

$$\int_i dv d\vec{r} \frac{1}{v} \frac{\partial \phi}{\partial t} = - \int_i dv d\vec{r} \frac{1}{v} \vec{v} \cdot \vec{\nabla} \phi \cdots \text{etc.} \quad (2)$$

The integrals may be replaced by the products of the volume of a cell and the average value of the function in the cell. The index i can be replaced by coarse variables, $\vec{R}$, $\vec{V}$, which are essentially identical to $\vec{r}$ and $\vec{v}$ except that they imply a macroscopic point of view. Finally, one obtains an equation identical to (1) in appearance.

$$\begin{aligned} \frac{1}{V} \frac{\partial \phi(\vec{R}, \vec{V})}{\partial t} = & - \frac{1}{V} \vec{V} \cdot \vec{\nabla} \phi(\vec{R}, \vec{V}) - \Sigma_t(\vec{R}, V) \phi(\vec{R}, \vec{V}) \\ & + \int d\vec{V}' \left[\frac{1}{4\pi} v_f(\vec{R}, V') \Sigma_f(\vec{R}, V') \chi_f(V) \right. \\ & \left. + \frac{1}{4\pi} v_{in}(\vec{R}, V') \Sigma_{in}(\vec{R}, V' \rightarrow V) + \Sigma_s(\vec{R}, V', \vec{V}' \cdot \vec{V}) \right] \phi(\vec{R}, V') \quad (3) \end{aligned}$$

in which the use of the variables $\vec{R}$ and $\vec{V}$ as arguments of a function implies that it is a local average.

Equation (3) is considerably simpler than (1) for two reasons. First, the cross sections vary slowly with position in the reactor and with energy and may be treated as constants over relatively large regions. Secondly, the fluxes vary slowly with position so that it is often satisfactory to replace (3) by the diffusion theory approximation to it.

The local averages used in Equation (3) are defined according to their use in (1)

$$\begin{aligned}\phi(\vec{R}, \vec{V}) &= \int_{\Delta V} dv \int_{\Delta \vec{r}} d\vec{r} \phi(\vec{r}, \vec{v}) / \Delta \\ \Sigma_t(\vec{R}, V) &= \left[\int_{\Delta V} dv \int_{\Delta \vec{r}} d\vec{r} \Sigma_t(\vec{r}, v) \phi(\vec{r}, \vec{v}) \right] / \phi(\vec{R}, \vec{V}) \Delta \quad (4)\end{aligned}$$

et cetera

where Δ represents the four dimensional cell volume.

For a generally cylindrical system, (3) may be integrated over two of the cylindrical coordinates θ and Z , so that an equation involving only one variable, R , the distance from the cylindrical axis is obtained:

$$\begin{aligned}\frac{1}{V} \iint \frac{\partial \phi(R, \theta, Z, \vec{V})}{\partial t} R d\theta dZ &= - \iint \frac{1}{V} \vec{V} \cdot \hat{R} \frac{\partial \phi(R, \theta, Z, \vec{V})}{\partial R} R d\theta dZ - \iint \Sigma_t(R, \theta, Z, V) \phi(R, \theta, Z, \vec{V}) R d\theta dZ \\ &+ \int d\vec{V}' \left[\frac{1}{4\pi} \iint \nu_f(R, \theta, Z, V') \Sigma_f(R, \theta, Z, V') \chi_f(V) R d\theta dZ \right. \\ &+ \frac{1}{4\pi} \iint \nu_{in}(R, \theta, Z, V') \Sigma_{in}(R, \theta, Z, V' \rightarrow V) R d\theta dZ \\ &+ \left. \iint \Sigma_s(R, \theta, Z, V', \vec{V}' \rightarrow \vec{V}) \phi(R, \theta, Z, \vec{V}') \right. \\ &\left. - \frac{1}{V} \vec{V} \cdot \hat{Z} \left[\int \phi(R, \theta, H, \vec{V}) R d\theta + \int \phi(R, \theta, -H, \vec{V}) R d\theta \right] \right] \quad (5)\end{aligned}$$

where $\hat{R}$ and $\hat{Z}$ are appropriate unit vectors.

The last term accounts for the leakage at the ends, $Z = \pm H$ of the reactor; actually H may be a function of R without affecting the validity of (5).

The appearance of Equation (5) may be simplified by replacing the integrals over θ and Z by quantities which have been averaged over these variables. Averaged quantities are indicated by underlining. On dividing by $4\pi RH$, one obtains,

$$\begin{aligned} \frac{1}{V} \frac{\partial \phi(R, \vec{V})}{\partial t} = & - \frac{1}{V} \vec{V} \cdot \hat{R} \frac{\partial \phi(R, \vec{V})}{\partial r} - \Sigma_t(R, V) \phi(R, \vec{V}) \\ & + \int d\vec{V}' \left[\frac{1}{4\pi} \nu_f(R, V') \Sigma_f(R, V') \chi_f(V) \right. \\ & + \frac{1}{4\pi} \nu_{in}(R, V') \Sigma_{in}(R, V' \rightarrow V) \\ & \left. + \Sigma_s(R, V', \vec{V}' \cdot \vec{V}) \right] \phi(R, \vec{V}') - L(R, \vec{V}) \end{aligned} \quad (6)$$

where

$$\begin{aligned} \phi(R, \vec{V}) &= \frac{1}{4\pi H} \int_{-H}^H dZ \int_0^{2\pi} d\theta \phi(R, \theta, Z, \vec{V}) \\ \Sigma_t(R, V) &= \int d\vec{\Omega} \frac{1}{4\pi H} \int_{-H}^H dZ \int_0^{2\pi} d\theta \Sigma_t(R, \theta, Z, V) \phi(R, \theta, Z, \vec{V}) \bigg/ \int d\vec{\Omega} \phi(R, \vec{V}) \\ L(R, \vec{V}) &= \frac{1}{4\pi H} \frac{1}{V} \vec{V} \cdot \hat{Z} \left[\int \phi(R, \theta, H, \vec{V}) d\theta - \int \phi(R, \theta, -H, \vec{V}) d\theta \right] \end{aligned} \quad (7)$$

et cetera

There is a minor approximation implied in (5) in that the flux used as a weighting function must be averaged over all directions of motion of the neutron in the calculation of Σ_s , but this approximation should not introduce appreciable errors.

Equation (6) and (7) show how a three space dimensional cylindrical reactor may be studied in terms of a one-space dimensional neutron transport equation if the behavior of the neutron flux as a function of the other spatial quantities

is known from other considerations. The usual one dimensional diffusion approximation may be obtained from Equation (6). As a result of the averaging carried out in (3) and (4), this approximation is broadly valid because of the slowly varying nature of the functions involved.

IV. GENERAL OUTLINE OF THE RBU METHOD

In RBU the calculation of the neutron flux is performed in two ways. Dependence on θ and Z and the rapid variation of neutron flux within small ranges of energy and small volumes -- microscopic variations -- are computed by the monte carlo method. The gross dependence of flux on energy and radial distance from the cylindrical axis is computed using diffusion theory; the associated fluxes, regions, and groups are called macroscopic. The cross sections for macroscopic calculations are obtained in a manner similar to that outlined above by using the microscopic fluxes as weighting functions. Diffusion coefficients are obtained from the monte carlo results as the ratio of the net current leaving a macroscopic region to the normal gradient of the neutron flux at the surface bounding that region. Using this definition of the diffusion coefficient instead of the standard one involving the transport mean free path makes the integral of the diffusion equation over a region agree identically with the integral of the transport equation over the same region, and thus extends the validity of the diffusion approximation. The monte carlo calculations may be performed separately on isolated portions of the reactor, each containing a number of microscopic regions; such a portion is called a monte carlo system. The relationship between separate monte carlo systems is established by imposing as a boundary condition the requirement that the ratio between the emergent and incident neutron currents at the surfaces bounding the monte carlo systems agree with values tabulated for each macroscopic energy group. These ratios, called albedoes in this report (although they may be greater than unity), are determined from the macroscopic fluxes. The relationship between separate monte carlo systems is further established by using the macroscopic fluxes as normalizing functions for the fluxes in the microscopic regions represented.

The program may be instructed to modify the contents of a sequence of specified microscopic regions sequentially so that the reactor remains just critical as determined by a diffusion calculation. In this case the program iterates between the adjustment routine and the diffusion calculation until criticality is achieved. When a satisfactory diffusion calculation has been completed, the program prepares to determine the change in isotopic concentrations in some microscopic regions resulting from the exposure in the time

steps which have taken place since the last burnup calculation on those regions. This involves the solution of a set of partial differential equations for isotope accretion and depletion. Not all microscopic regions are "burned up" after each time step. The number of time steps -- that is, diffusion calculations -- between burnups is determined for each material by comparing the difference between two estimates of the concentrations with an upper and lower error tolerance limit. The program will thus adjust the time steps represented by burnup calculations for each material and, occasionally, will also adjust the time intervals represented by the diffusion calculations.

When the isotopic concentrations in a region and, consequently, the microscopic fluxes have changed sufficiently to appreciably alter the effective average cross sections it is desirable to repeat the monte carlo calculations to obtain new microscopic fluxes. The number of diffusion time steps between monte carlo calculations is specified by a number given as input for each monte carlo system.

The program continues cyclically -- consuming and accumulating isotopes, computing fluxes by diffusion theory to use in the isotope accretion and depletion calculation and re-evaluating the microscopic fluxes to use as weighting functions for the diffusion equations -- until an indication is reached that the calculation should be stopped. This indication is that either the maximum possible adjustments have been made in the compositions of all the microscopic regions in the sequence of control regions, or that the time variable has reached a predetermined value.

The general outline just described is shown as a flow chart in Figure 1.

In addition to the programming described in Figure 1, there are two auxiliary codes: a cross section averaging routine which produces data for the isotopes required from a basic cross section library; and an editing routine which collects selected output information and prepares it for off-line printing.

Figure 1

OVER-ALL FLOW CHART OF RBU

*Refers to quantities described on Page 19

V. THE MONTE CARLO PORTION OF RBU

The RBU monte carlo is essentially similar to a previous monte carlo program, GMC. Modifications have been introduced in order to improve the speed and versatility of the program and to extend the treatment of such phenomena as resonances, neutron thermalization and anisotropic scattering.

A. GEOMETRY

The geometric description of a monte carlo system is made by first specifying the parameters of the set of B surfaces bounding the regions in the system. A surface is identified by the index b. The surfaces which the program recognizes are of the form

$$A(x-x_0)^2 + B(y-y_0)^2 + C(z-z_0)^2 - K = 0 \quad (8)$$

In order to increase computing speed, certain special cases of (8) are specifically provided for. These are

$$(x-x_0)^2 + (y-y_0)^2 - K = 0 \quad (9)$$

$$x - K = 0 \quad (10)$$

$$y - K = 0 \quad (11)$$

$$z - K = 0 \quad (12)$$

Surfaces are specifically assigned one of the forms (8), (9), (10), (11), or (12) by associating with them a value of an index D_b of 0, 1, 2, 3, or 4 respectively.

A microscopic region of space, h , is defined by listing the indices (values of b) for the surfaces bounding it. For each of these surfaces it is also necessary to specify whether an index g_{b_h} has the value plus or minus one. A surface b_h of region h has a positive value of g_{b_h} if the boundary function r_b is negative for values of the coordinates x , y , and z within region h with respect to boundary b . The term g_{b_h} is negative if r is positive for values of x , y , and z inside region h with respect to b .

The boundary function is defined by one of the following equations depending on the value of D.

$$r = \begin{cases} A(x-x_0)^2 + B(y-y_0)^2 + C(z-z_0)^2 - K \\ (x-x_0)^2 + (y-y_0)^2 - K \\ y - K \\ x - K \\ \text{or} \\ z - K \end{cases} \quad (13)$$

Additional quantities associated with a region are an index m_h , specifying the material contained in region h ; a value of I_h , the importance of region h ; k_h , the macroscopic region within which h is contained; B_h , the total number of bounding surfaces used to describe h ; $\perp_{b_h}$, which indicates whether or not boundary b of region h is part of the top or bottom surface of the reactor and, therefore, whether or not leakage from region h through boundary b contributes to the perpendicular leakage to be used for region k_h in the diffusion calculation; and q_{b_h} , q'_{b_h} , indices of the microscopic regions (in order of likelihood) which a neutron leaving region h through boundary b will probably enter.

Region h belongs to a set, f_h , of microscopic regions. The neutron fluxes computed in the monte carlo are listed as the fluxes, ϕ_{if} in group i , region set f .

B. DESCRIPTION OF A MATERIAL

As mentioned above, the description of a region, h , includes an index, m_h , which determines which of the M mixtures of isotopes is contained in region h . The information about a material required by the monte carlo portion of RBU is collected and computed from a basic detailed library of isotopic properties, and from the input by two portions of the program, the Cross Section Averaging Routine and the Pre-Monte Carlo. These portions of the program, described in later sections of this report, assemble the

nuclear data for each material and each microscopic energy group, i . In brief these data consist of mean free paths, λ_{mi} ; emission probabilities for the pertinent collision types, $P_{c_{mi}}$; atomic weights of the scatterers, A_{mi} ; prescriptions for the inelastic scattering spectra; probability distributions for velocity increments for near thermal scattering; parameters for the resonances for those scatterers in the material which have them; and finally coefficients for anisotropic scattering.

C. GENERAL OUTLINE OF THE MONTE CARLO PORTION

Particles - that is, the position, velocity, and time coordinates of particles - are followed for an interval of time from 0 to T or until they are terminated before T by capture or by escape from the system. The determination of variables, such as distance between collisions and directions and velocities after collision is made by random selection from the relevant probability distributions. At each collision, analytic calculations are made of the values of certain averages for a universe of neutrons with the coordinates with which particles emerge from the collision. These averages are the first flight contributions for the monte carlo time interval of such quantities of interest as the neutron flux in each microscopic group, i , and region set, f , and the currents and normal gradients of the currents at the boundaries of macroscopic regions in each macroscopic group. Thus, the monte carlo method is used to establish a collision distribution from which the quantities of interest are computed analytically. To each microscopic group and region an importance is assigned by the input; the number of neutrons represented by a particle in region h and group i is $\frac{1}{I_i I_h}$, the reciprocal of the product of the importances of the group and region in which it is. Since neutrons are conserved when particles cross from one group or region to another, the effect of this is to make the intensity with which a group and region is studied a function of its importance as well as of the actual neutron population.

The particles to be studied are obtained initially from a tape containing those which reached census time, T , in the previous monte carlo time step for this system. For the first time step, of course, they must be obtained elsewhere; they may either be particles saved from previous calculations or particles generated by a special generator routine.

A period of time between 0 and T_0 , during which the particles are followed without recording their history, is inserted in order to permit the population to come into equilibrium with the configuration of the system. In order to accelerate this process, the number of particles in each region and group actually used is modified from that on the tape of initial particles according to the variation in flux between previous monte carlo calculations of this system.

D SAMPLING FROM INITIAL NEUTRON TAPE

On reading a particle from the initial neutron (I.V.)^{*} tape, the program first checks to be sure that the region h indicated by its coordinates is actually the region in which the particle is located.

The condition that a particle be in zone h is that, for all boundaries, b_h of h

$$g_{b_h} \cdot r_{b_h}(x,y,z) \leq 0 \quad (14)$$

The method used to determine whether or not a set of coordinates lies within a region imposes a limitation on the possible region shapes. Generally speaking this is that no two boundaries of a region may meet in such a way as to produce a concavity. This does not affect the generality of the geometry since a set of regions may have any shape. If the particle is not in zone h , the program tests all other regions to determine which region it is in.

The procedure of checking to be sure that a particle read from the I.V. tape is actually in the indicated zone is inserted in order to make it possible to interchange I.V. tapes between problems. During the normal operation of RBU and in particular after the first monte carlo time step,

^{*}I.V. is an abbreviation for initial value.

the zone index associated with a particle may be assumed to be correct. The program, in fact, will insist upon this and will bypass the zone checking routine unless sense switch 3 has been depressed.

Having determined the correct region number and substituted this for h , the program next decides how many times this set of initial coordinates is to be followed. Included in a set of coordinates is a number, N , the number of particles having the exact values of x , y , z , V , α , β , and γ , given in that set. The term N , in other words, is the number of particles represented by a set of coordinates. The fact that N may be different from unity is a result of the sampling procedure about to be described and of the manner in which particles come to be written on the census tape. The modification of N , on reading a set of coordinates from the I.V. tape is made to accomplish two purposes. First, the distribution of particles on the I.V. tape is to be distorted in order to accelerate the approach to equilibrium. This introduces a factor A_{ih}^t in the number of particles to be made of the particle read from the I.V. tape. (The superscript t indicates the monte carlo time step number.) Secondly, the total number of particles to be followed is to be adjusted to approximate the number, N_{MC} which the programmer considers to be necessary for the required statistics. N , then, is changed to

$$\left[A_{ih}^t \frac{N_{MC}}{N_{I.V.}^t} N + \xi \right] \quad (15)$$

The symbol $\left[\right]$ signifies "greatest integer in" and ξ is a random number (see Appendix B). By adding a random number and taking the greatest integer, the program selects integral values of quantities in such a way that the average of many such selections approaches the appropriate number -- in this case

$$A_{ih}^t \frac{N_{MC}}{N_{I.V.}^t} N$$

The term $N_{I.V.}^t$ is the total number of particles on the I.V. tape. It may be assumed to be equal to the number of particles which reached census time in the previous monte carlo time step.

E. UNRESOLVED RESONANCES

The next stage of the monte carlo program involves the knowledge of the mean free paths in the region in which the particle has just been found to be. In most cases this is obtained from tables prepared in the pre-monte carlo routine. Some materials, however, contain isotopes the cross sections of which are, for part of the energy range of interest, most conveniently described by parameters specifying distributions of single level Breit Wigner resonances. These parameters are

D , the mean energy between resonances in e.v.

$\bar{\Gamma}_{no}$, the mean reduced neutron partial width in (e.v.)^{1/2}

$\bar{\Gamma}_f$, the mean fission partial width in e.v.

Γ_γ , the partial radiative capture width in e.v.

σ_p , the potential scattering cross section in barns

g , the statistical weight

I_3 and I_2 , the upper and lower inclusive limits of the groups in which the unresolved resonances cross sections are used

N , the atomic concentration of the pertinent isotope in atoms per cm³

The values of these are specified for each of the resonance isotopes in the region. For each of these isotopes the actual value of the cross sections seen by a particle at an individual event is determined by random selection from the appropriate probability distributions. The probability that

$$u \equiv \left(\frac{\Gamma_{no}}{\bar{\Gamma}_{no}} \right)^{1/2} \quad (16)$$

be between u and $u + du$ is given by the Porter-Thomas distribution

$$\frac{dP(u)}{du} du = \sqrt{2/\pi} e^{-u^2/2} du \quad (17)$$

and the probability that

$$v \equiv \Gamma_f / \bar{\Gamma}_f \quad (18)$$

be between v and $v + dv$ is

$$\frac{dP(v)}{dv} dv = e^{-v} dv \quad (19)$$

The manner in which values of Γ_{n_o} and Γ_f are selected from these distributions is described in Appendix B; Γ_γ is assumed to be constant for all unresolved resonances for a particular isotope.

The cross section at E , the energy of the neutron, is approximated by the sum of that contributed independently by two resonances whose peaks lie at

$$E_{o_a} = \left[\frac{V^2}{1.916 D} \right] D \text{ and}$$

$$E_{o_b} = E_{o_a} + D \quad (20)$$

where V is the neutron velocity in cm/microsecond. Values of the partial widths are selected for each of the two resonances as described above and the cross section due to each is evaluated from

$$\Gamma_{n_o} \sqrt{E_o} \quad \text{in e.v.}$$

$$\Gamma = \Gamma_\gamma + \Gamma_f + \Gamma_n, \quad \text{in e.v.}$$

$$\theta = 1.798 \times 10^{-4} \frac{V^2 T}{a \Gamma^2} \left(\frac{a}{a+1} \right)^2 \quad (\text{dimensionless})$$

$$X = 2 \left[\frac{V^2}{1.916} \frac{a}{a+1} - E_o \right] / \Gamma \quad (\text{dimensionless}) \quad (21)$$

where a is the mass number of the resonance isotope and T is the temperature of the material in degrees Kelvin; from

$$\sigma_{s_o} = 2.607 \times 10^6 \text{ g} \left(\frac{1+a}{a} \right) \frac{\Gamma_n^2}{E_o \Gamma^2} (1+4.27 \times 10^{-7} V^2) (1+1.42 \times 10^{-3} V) \quad (\text{barns})$$

$$\sigma_{c_o} = 3.608 \times 10^6 \text{ g} \left(\frac{1+a}{a} \right)^{3/2} \frac{1}{V \sqrt{E_o}} \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} (1+4.27 \times 10^{-7} V^2) (1+1.42 \times 10^{-3} V) \quad (\text{barns})$$

$$\sigma_{f_o} = 3.608 \times 10^6 g \left(\frac{1+a}{a} \right)^{3/2} \frac{1}{v\sqrt{E_o}} \frac{\Gamma_n \Gamma_f}{\Gamma^2} (1+4.27 \times 10^{-7} V^2) (1+1.42 \times 10^{-3} V) \text{ (barns)}$$

and from

$$\begin{aligned} \sigma_s &= \sigma_{s_o} \psi(X, \theta) + 2 \sqrt{\sigma_p g \sigma_{s_o}} \chi(X, \theta) + \sigma_p \text{ (barns)} \\ \sigma_c &= \sigma_{c_o} \psi(X, \theta) \text{ (barns)} \\ \sigma_f &= \sigma_{f_o} \psi(X, \theta) \text{ (barns)} \end{aligned} \quad (22)$$

The factors $\frac{D'}{D} = 1 + 4.27 \times 10^{-7} V^2$ and $\ell^* = 1 + 1.42 \times 10^{-3} V$ are rough approximations included to account for the variation of level density with energy and for the presence of resonances with angular momentum higher than $\ell = 0$. The broadened resonance functions are defined by

$$\begin{aligned} \psi(X, \theta) &= \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{e^{-\left[\frac{(X-Y)^2}{4\theta}\right]}}{1+Y^2} dY \\ \chi(X, \theta) &= \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{Y e^{-\left[\frac{(X-Y)^2}{4\theta}\right]}}{1+Y^2} dY \end{aligned} \quad (23)$$

The evaluation of ψ and χ is described in Appendix C and the derivation of (22) and (23) is described in Appendix D.

F. RESOLVED RESONANCES

Resolved resonances are treated in a manner similar to that described above for unresolved resonances. The difference is that the values of the parameters, E_o , Γ_n , and Γ_f are specified. For neutrons in velocity groups between I_{3wm} and I_{2wm} , the cross sections for the w^{th} resonance scatterer in material m are computed using Equation (22) with values of E_o , Γ_n , Γ_f , g , and Γ_f obtained from one of the lists of resonance parameters stored in the memory. An index associated with the w^{th} resonance scatterer of material m identifies the list to be used for it. As in the unresolved region, the cross sections computed are the sum of independent contributions of two

resonances, these being the ones with values of E_0 on either side of the energy, $\frac{v^2}{1.916}$ of the neutron. The values of the other resonance parameters are the same as those used in the unresolved region for the same scatterer.

G. BETWEEN COLLISIONS ROUTINE

In this stage of the calculation a group of N particles, each having identical coordinates, which have resulted either from a collision or from selection from the I.V. tape, are followed to their individual next collisions, to census time, or to loss, through leakage, from the system. In the course of this process, the expectation values of the contributions of these particles to quantities of interest are computed region by region for the entire path the particles have the possibility of following in first flight until they leak or reach census time. The distance a particle at position x, y, z traveling in direction α, β, γ will have to go to reach boundary b of region h is

$$S_b = \frac{-e + g_{bh} \sqrt{e^2 - hr}}{h} \quad (24)$$

where

$$\begin{aligned} e &= A_{bh} \alpha(x - x_{obh}) + B_{bh} \beta(y - y_{obh}) + C_{bh} \gamma(z - z_{obh}) \\ h &= A_{bh} \alpha^2 + B_{bh} \beta^2 + C_{bh} \gamma^2 \\ r &= A_{bh} (x - x_{obh})^2 + B_{bh} (y - y_{obh})^2 + C_{bh} (z - z_{obh})^2 - K_{bh} \end{aligned} \quad (25)$$

For the special boundaries of Equations (9) through (12) these formulas reduce to

$$\left. \begin{aligned} e &= \alpha \left(x - x_{o_{bh}} \right) + \beta \left(y - y_{o_{bh}} \right) \\ h &= \alpha^2 + \beta^2 \\ r &= \left(x - x_{o_{bh}} \right)^2 + \left(y - y_{o_{bh}} \right)^2 - K_{bh} \end{aligned} \right\} \quad D = 1 \quad (26)$$

$$S_b = - \frac{x-K}{\alpha} \quad \text{if} \quad \frac{x-K}{\alpha} < 0 \quad (D=2)$$

$$S_b = - \frac{y-K}{\beta} \quad \text{if} \quad \frac{y-K}{\beta} < 0 \quad (D=3)$$

$$S_b = - \frac{z-K}{\gamma} \quad \text{if} \quad \frac{z-K}{\gamma} < 0 \quad (D=4) \quad (27)$$

The distance to boundary is computed by means of one of Equations (24) through (27) for each of the boundaries of the region in which the particle is, the smallest positive value so obtained being accepted as the actual distance. In order to minimize computing time on calculations involving (24) (that is when $D_b = 0$ or 1), Sturm's Theorem of the locations of roots of a quadratic equation is used to decrease the number of boundaries for which the calculation is actually made.

The between collisions routine begins with a set of N particles at a particular position and with a particular velocity. These represent $\frac{N}{I_i I_h}$ neutrons where I_i and I_h are the importance of group i and the importance of region h respectively. By random selection from the appropriate distribution, a distance to collision is determined for each of the N particles. These are the distances each will go before having a collision provided it does not first cross a boundary into a new region or reach census time. For each of those particles which have a collision before leaving the region, the program transfers to the collision routine, computes the new velocity and direction, and stores the coordinates of the resultant particles in a region of memory known as born storage. At an appropriate stage of the program, they will be followed further. The remaining particles (those which have not had collisions in the region in question) are advanced just over the boundary into the next region,

provided they do not first reach census time, and N is diminished by the number which had failed to reach the boundary. Associated with this set of particles is a number, $\prod$ representing the expectation value of the number of neutrons of the set reaching the region in which they are being considered. This is initially set to $\frac{N}{I_h I_i}$ when the set of particles is obtained from born storage or the I.V. tape, and is diminished by the factor $e^{-S_b/\lambda}$ each time the program advances the particles a distance S_b through a region.

The expectation value of the path length (which is, of course, proportional to the flux) swept out by particles starting at a distance S from the boundary of a region is

$$\phi_{if} = \lambda \prod (1 - e^{-S/\lambda}) \quad (28)$$

Since the quantity of interest here, however, is the track length during the period $T_0 \leq t \leq T$, (28) is modified by using for S the distance the particle could possibly travel in that period in region h and by multiplying by the attenuation taking place during the period (if any) during which $t < T_0$. Thus

$$\phi_{if} = \lambda \prod p_1 (1 - p_2) \quad (28a)$$

where

$$p_1 = \begin{cases} \exp - \left[\frac{(T_0 - t)V}{\lambda} \right] & \text{if } t < T_0 \text{ and } (T_0 - t)V < S_b \\ 0 & \text{if } t < T_0 \text{ and } (T_0 - t)V \geq S_b \\ 1 & \text{if } t \geq T_0 \end{cases}$$

$$p_2 = \begin{cases} e^{-S_b/\lambda} & \text{if } (T - t)V \geq S_b \text{ and } t \geq T_0 \\ e^{-(T-t)V/\lambda} & \text{if } (T-t)V < S_b \text{ and } t \geq T_0 \\ e^{-(T-T_0)V/\lambda} & \text{if } (T-t)V < S_b \text{ and } t < T_0 \\ e^{-[S_b - (T-T_0)V]/\lambda} & \text{if } (T-t)V \geq S_b \text{ and } t < T_0 \end{cases} \quad (29)$$

The average cross sections to be used in the diffusion and burnup calculations for the isotopes having resonances are obtained from expectation value calculations also. For a particle in macroscopic group j in a region containing material m , the appropriate tallies for the w^{th} resonances isotopes of material m are

$$\begin{aligned}(\Sigma_s \phi)_{w_m j} &= \prod p_1 (1-p_2) \Sigma_s \lambda \\(\Sigma_f \phi)_{w_m j} &= \prod p_1 (1-p_2) \Sigma_f \lambda \\(\Sigma_c \phi)_{w_m j} &= \prod p_1 (1-p_2) \Sigma_c \lambda\end{aligned}\quad (30)$$

For particles crossing from one macroscopic region to another, the expectation value of the components of the neutron current and of the gradient of the neutron flux normal to the interface between these regions are also tallied. These tallies are used to compute the diffusion coefficients. The appropriate quantities for particles reaching the interface between macroscopic regions k and k' in macroscopic group j are

$$\begin{aligned}L_{kj} &= \prod (1-\omega_{bj}) = -L_{k'j} \\(\hat{n} \cdot \vec{\nabla} \phi)_{kj} &= \prod \frac{(1-\omega_{bj})}{\nabla^2} \left[\frac{gh}{(e^{-2hr})^{1/2}} - \frac{1}{\lambda} \right] = -(\hat{n} \cdot \vec{\nabla} \phi)_{k'j} \\ \nabla &= \lambda + \delta + \rho\end{aligned}\quad (31)$$

where λ is the mean free path for the microscopic group and region in which the particle is when it reaches the boundary, ω_{bj} is the albedo for boundary b and macroscopic group j .

$$\begin{aligned}\lambda &= A \alpha(x-x_0) / \mathcal{S} \\ \delta &= B \beta(y-y_0) / \mathcal{S} \\ \rho &= C \gamma(z-z_0) / \mathcal{S} \\ \mathcal{S} &= \left[\alpha^2 A^2 (x-x_0)^2 + \beta^2 B^2 (y-y_0)^2 + \gamma^2 C^2 (z-z_0)^2 \right]^{1/2}\end{aligned}\quad (32)$$

A, B, C, x_0, y_0, z_0 are the parameters for the relevant boundary. For boundaries of the special forms, $D = 2, 3$ or 4 , (31) simplifies to

$$(\hat{n} \cdot \vec{\nabla} \phi)_{kj} = \prod \frac{1}{\Delta \lambda} \frac{(1-\omega_{bj})}{(\alpha, \beta \text{ or } \gamma)} = -(\hat{n} \cdot \vec{\nabla} \phi)_{k'j}$$

while the simplified forms of (32) are:

$$\begin{aligned}
 D = 1 \quad \kappa &= \alpha(x-x_0)/\rho \\
 \delta &= \beta(y-y_0)/\rho \\
 \rho &= 0 \\
 \rho &= [(x-x_0)^2 + (y-y_0)^2]^{1/2} \\
 D = 2 \quad \kappa &= \alpha \\
 \delta &= \rho = 0 \\
 D = 3 \quad \delta &= \beta \\
 \kappa &= \rho = 0 \\
 D = 4 \quad \kappa &= \rho = 0 \\
 \rho &= \gamma
 \end{aligned} \tag{33}$$

The expectation value of the leakage out of the system from microscopic region h through boundary b_h is tallied separately for those region-boundary combinations for which the quantity $\perp_{b_h}$ in the input is non-zero. These tallies, used to obtain the perpendicular leakage term in Equation (6), are recorded by macroscopic region and group

$$L_{kj} = \prod (1 - \omega_{bj}) \tag{34}$$

When the monte carlo program is used as a part of RBU, it will generally be true that ω_{bj} is zero for any boundary for which $\perp_{b_h}$ is not zero and vice versa.

Certain other quantities are also computed, some of these primarily for code and input checking purposes.

$N_{I.V.}$	: Number of initial neutrons followed
$\mathcal{N}_{I.V.}$	: Number of initial particles followed
$N_{C.V.}$	: Number of neutrons reaching census
$\mathcal{N}_{C.V.}$	: Number of particles reaching census
$\langle N_{BO} \rangle$	: Expectation value of the number of neutrons escaping from the system by leakage
N_{BO}	: Number of neutrons escaping from the system by leakage

- N_B : Net number of neutrons lost at internal boundaries
 (due to statistical fluctuations associated with the
 use of weights)
 N_{BW} : Number of neutrons lost at albedo surfaces
 $\langle N_c \rangle$: Expectation value of the number of neutrons
 entering collisions
 $\langle Ne' \rangle$: Expectation value of the number of neutrons emerging
 from collisions
 Ne : Number of neutrons emerging from collision

These are the quantities referred to as "code check quantities" in Figure 1

As described above, for each particle a determination is made individually of whether or not the particle is to have a collision before reaching the boundary of the region it is crossing. The determination is made by random selection of S_c from the distribution

$$\frac{dP(S_c)}{dS_c} = \frac{1}{\lambda} e^{-S_c/\lambda} \quad (35)$$

For each particle for which S_c is less than both S_b and $S_T = (T-t)V$, the program transfers to the collision routine in which the results of the collision are determined. The coordinates of any particles emitted in the collision are stored temporarily in a region of memory known as born storage and the program returns to the between collisions routine to process the remaining particles and the remainder of the undeflected path.

H. COLLISION ROUTINE

Among the material data, as was mentioned previously, is a set of numbers, $P_{c_{mi}}$, the number of neutrons produced due to collision process c per neutron colliding in material m and microscopic group i . The different values of the index c correspond to the different collision types, elastic, inelastic, and fission and where necessary (as in the case of elastic collisions with light nuclei and inelastic collisions

where the scatterers present have different inelastic scattering spectra) to the different isotopes present.

On entering the collision routine the program determines whether or not to select new coordinates for particles to be emitted by a collision process. This decision depends on whether or not

$$N' = \left[P_{c_{mi}} + \xi \right] \quad (36)$$

is zero.

The program then proceeds, if $N' \neq 0$, to determine the direction and velocity of the emergent particles by methods dependent on the collision type and to be described below. In the event that a change in velocity takes place, it may be necessary to modify N' when the new velocity is known because of the group weights. If I_i and I_i' are respectively the importance of the group in which the particle is incident and that of the one in which it emerges

$$N = \left[\frac{I_i'}{I_i} N' + \xi \right] \quad (37)$$

If N is not zero the particle's coordinates are stored in born storage and the program considers the collision corresponding to the next value of c .

Radiative capture collisions are automatically accounted for in this process by their effect in diminishing the value of $\sum_c P_{c_{mi}}$. The other collision types will now be discussed.

1. Elastic Scattering

The simplest case for elastic collisions occurs for heavy scatterers when the energy of the incident neutron is below the minimum (specified by I_{aniso}) for anisotropic scattering and when it is not in a range in which moderation by heavy nuclei is considered. Under these circumstances, that is when

$$\begin{aligned}
a_r &> a_H \\
I_{H_{1m}} &> i \text{ or } i > I_{H_{2m}} \\
i &> I_{\text{aniso}_r}
\end{aligned} \tag{38}$$

the neutron's velocity does not change. The emergent direction cosines are selected at random from an isotropic universe as described in Appendix B. In (38), a_r is the atomic weight of the scatterer; a_H is the atomic weight defining light and heavy scatterers; I_{aniso_r} is the lowest energy group (highest group number) in which anisotropic scattering is considered for r^{th} scatterer and $I_{H_{1m}}$ and $I_{H_{2m}}$ are the upper and lower energy group limits (lower and upper group numbers) of the range in which heavy scatterers are permitted to moderate the neutrons.

If either of the first two conditions of (38) fail, the relationship between the center of mass and laboratory systems must be taken into account. In the isotropic case, random direction cosines α'' , β'' , and γ'' are chosen from an isotropic distribution and the value of μ , the cosine of the angle between the incident and emergent directions in the center of mass system is determined.

$$\mu = \alpha\alpha'' + \beta\beta'' + \gamma\gamma'' \tag{39}$$

The emergent direction cosines in the laboratory system, α' , β' , γ' , and the emergent velocity V' are then calculated from

$$\begin{aligned}
\alpha' &= (a_r \alpha'' + \alpha)/C \\
\beta' &= (a_r \beta'' + \beta)/C \\
\gamma' &= (a_r \gamma'' + \gamma)/C \\
V' &= VC/(1 + a_r)
\end{aligned} \tag{40}$$

where

$$C = [1 + a_r^2 + 2\mu a_r]^{1/2}$$

In order to conserve computing time and storage space for the $P_{c_{mi}}$, the same value of a_r is used for all heavy scatterers in (40).

This permits the lumping of all heavy scatterers in one value of c . The atomic weight normally used for these is 238.

When scattering is anisotropic, that is when $i < i_{\text{aniso}}$, a simple modification causes the selection of the angle of scattering in the center of mass system to be made from

$$\frac{dP(\mu)}{d\mu} = a_0 + a_1\mu + a_2\mu^2 + a_3\mu^3 \quad (41)$$

The method is to compute μ from

$$\mu = \alpha\alpha'' + \beta\beta'' + \gamma\gamma'' \quad (42)$$

as above, but to accept the random cosines α'' , β'' , γ'' only if

$$\xi a_m \leq a_0 + a_1\mu + a_2\mu^2 + a_3\mu^3 \quad (43)$$

In (43), ξ is a number chosen at random from a uniform distribution between zero and one. If (43) is not satisfied by μ and ξ , a new set α'' , β'' , γ'' , ξ are chosen. Thus, the probability of accepting a direction is proportional to (41). The values of a_0 , a_1 , a_2 , a_3 , and a_m used in (43) are found in the listings of material data separated according to microscopic energy group and scatterer. The term a_m is the largest possible value of $dP(\mu)/d\mu$ for $-1 \leq \mu \leq 1$ and is computed in the portion of the program in which the monte carlo constants are calculated. For the collective heavy scatterer in a material only one set of a_i is stored for each group, this being a concentration and cross section weighted average over the heavy scatterers present computed by the pre-monte carlo portion of the program.

If moderation is unimportant α'' , β'' , γ'' are used as the new laboratory system direction cosines; if it is to be considered, as determined by the first two of Equations (38), α'' , β'' , and γ'' are used to compute the laboratory system direction cosines and velocity by (40).

When the energy of the particle is comparable with the thermal kinetic energy of the scattering nuclei, two further modifications are made in order to account for the effect of molecular and

crystal binding of the scattering atoms and the effect of their thermal motion. The first of these is that, if the emergent velocity in the center of mass system is less than V_T , the atomic weight used in (40) is permitted to vary with the incident microscopic group. Secondly, the new velocity in the center of mass system is modified by adding to it an incremental velocity $\Delta\vec{V}$. The magnitude of $\Delta\vec{V}$ is chosen by random selection from one of the probability distribution tables stored in memory for this purpose. An index associated with the scatterer determines which table is to be used. The direction cosines of $\Delta\vec{V}$, α''' , β''' , and γ''' , are selected at random from an isotropic distribution and finally the emergent velocity is

$$\begin{aligned}
 v_e &= \left\{ \Delta V^2 + 2 \frac{V\Delta V}{a+1} \left[\alpha''' (a\alpha'' + \alpha) + \beta''' (a\beta'' + \beta) + \gamma''' (a\gamma'' + \gamma) \right] \right. \\
 &\quad \left. + \left[a^2 + 1 + 2a(\alpha\alpha'' + \beta\beta'' + \gamma\gamma'') \right] \frac{v^2}{(a+1)^2} \right\}^{1/2} \\
 \alpha_e &= \frac{\frac{V}{a+1} (a\alpha'' + \alpha) + \Delta V \alpha'''}{v_e} \\
 \beta_e &= \frac{\frac{V}{a+1} (a\beta'' + \beta) + \Delta V \beta'''}{v_e} \\
 \gamma_e &= \frac{\frac{V}{a+1} (a\gamma'' + \gamma) + \Delta V \gamma'''}{v_e}
 \end{aligned} \tag{44}$$

When moderation is not significant, (44) reduces to a simpler set of equations.

2. Inelastic Scattering

Inelastic scattering in this program is assumed to be isotropic in the center of mass system. Although this may not always be the case in nature, neither the experimental data nor the importance of the effect justify including anisotropic inelastic scattering in the program at this time. Should the situation change in the future, the appropriate modifications can easily be made.

The emergent velocity in the center of mass system is chosen either from the evaporation model spectrum or from one of the probability distribution tables stored in the memory for this purpose. The program determines whether to use the evaporation model or, if not, which table to use by the value of a number D which is part of the data stored with each isotope in the basic library of data. If D is an integer between zero and 9, it is interpreted as the name of the appropriate inelastic spectrum table; otherwise, it is interpreted as the resonance spacing to be used in the evaporation model.

Using the evaporation model the emergent velocity V' is chosen from

$$\frac{dP(V')}{dV'^2} = CV'^2 e^{-V'^2/T_N}$$

$$T_N \equiv DV \quad (45)$$

V is the incident velocity of the neutron and C is a normalization constant.

The method of selecting from this distribution is described in Appendix B.

When the inelastic spectrum is determined by one of the probability distribution tables the method is to compare a random number ξ successively with the probabilities p_i , of the table to find the pair for which

$$p_i < \xi \leq p_{i+1} \quad (46)$$

The emergent velocity in the center of mass system is then

$$V'' = [V^2 - V_i^2]^{1/2} \quad (47)$$

provided the value so obtained is positive. To assure that it will be, ξ is drawn from a (uniform) distribution between zero and the entry, p_j , in the probability table such that

$$V_j^2 \leq V^2 < V_{j+1}^2 \quad (48)$$

In these equations, V_i^2 is the table velocity entry corresponding to probability, p_i and V_j^2 that corresponding to p_j . In this way the table is used to select an energy loss (proportional to V_i^2) according to the inelastic γ ray spectrum.

If the atomic weight of the scatterer is high, that is if

$$a > a_H$$

the center of mass velocity and direction is used for the laboratory system values. Otherwise the laboratory system values V' , α' , β' , γ' are computed by adding vectorially the velocity of the center of mass system.

$$\begin{aligned}
 V' &= \left[V''^2 + V^2 \left(\frac{1}{a+1} \right)^2 + 2V''V \frac{\alpha\alpha'' + \beta\beta'' + \gamma\gamma''}{a+1} \right]^{1/2} \\
 \alpha' &= (V''\alpha'' + \frac{V\alpha}{1+a})/V' \\
 \beta' &= (V''\beta'' + \frac{V\beta}{1+a})/V' \\
 \gamma' &= (V''\gamma'' + \frac{V\gamma}{1+a})/V'
 \end{aligned} \tag{49}$$

and (47) is modified to

$$V'' = \left[V^2 \left(\frac{a}{1+a} \right)^2 - V_1^2 \right]^{1/2} \tag{50}$$

Since it is assumed that the evaporation model spectrum will only be used for heavy nuclei, no provision is made for using the center of mass system incident velocity in (47). In the use of the inelastic spectrum tables, the approximation has been made that the spectrum of γ particles emitted is independent of the incident energy except that it has been truncated to prevent the emission of neutrons at negative energies.

3. Fission

Fission neutrons are assumed to be isotropically emitted. The emergent velocity is obtained by random selection from the fission spectrum table, (p_n, V_n^2) . A random number, ξ , is compared with the successive p_n to obtain an n such that

$$p_n \leq \xi \leq p_{n+1} \tag{51}$$

Then

$$V^2 = V_n^2 + \frac{\xi - p_n}{p_{n+1} - p_n} (V_{n+1}^2 - V_n^2)$$

Thus V is obtained by linear interpolation in the square of V from the fission spectrum tables.

I. CENSUS TIME

For those particles for which S_T , the distance to census time, is less than S_c or S_b the coordinates are advanced to the position at which $t = T$. That is

$$\begin{aligned}x + \alpha(S_T - \delta) &\rightarrow x \\y + \beta(S_T - \delta) &\rightarrow y \\z + \gamma(S_T - \delta) &\rightarrow z \\0 &\rightarrow t\end{aligned}\tag{52}$$

and the new coordinates are written on the census tape with a value of N equal to the number of particles of the set for which $S_T < (S_c, S_b)$. In (52) δ is a negligibly small number used whenever a particle is advanced to a new position to assure that round off errors do not place the particle in a different region from the anticipated one.

J. REFLECTION AT OUTER BOUNDARIES

When a particle is advanced, in the between collisions routine, to an outer boundary of the system it may be reflected back into the system. The reflection coefficient or albedo, ω_{bj} , a function of boundary and of macroscopic group, may have any positive value. It is computed from the macroscopic fluxes by Equation (63). On reflection, the value of $\bar{I}$, the intensity of the expectation beam is multiplied by ω_{bj} , while the number of reflected particles, N' , is obtained from the incident number, N , by

$$N' = \left[N \omega_{bj} + \xi \right]\tag{53}$$

The direction cosines α' , β' , γ' are computed from the relations

$$\begin{aligned}\alpha' &= \alpha - 2\kappa \frac{\nabla}{\alpha} \\ \beta' &= \beta - 2\delta \frac{\nabla}{\beta} \\ \gamma' &= \gamma - 2\rho \frac{\nabla}{\gamma}\end{aligned}\tag{54}$$

where κ , δ , ρ , and ∇ are defined by (31) and (32) or (33) with x, y, z , the point at which the particle hits the boundary and α , β , and γ the incident direction.

K. NORMALIZATION OF THE MONTE CARLO RESULTS

The monte carlo fluxes are not flux densities but total neutron track lengths per group and per region set. At the completion of the monte carlo calculation, they are normalized to a total flux of unity by division by

$$\sum_i \sum_{f \text{ in } k} \phi_{if}$$

The resonance collision tallies, $(\Sigma\phi)_w$ are normalized by division by $\sum_{\substack{i \text{ in } j \\ f \text{ containing } m}} \phi_{if}$.

The current and normal current gradient tallies need not be normalized since it is their ratio that is used in RBU. To facilitate use of the monte carlo portion for other purposes, however, they are normalized by division by $\sum_{\substack{i \text{ in } j \\ f \text{ in } k}} \phi_{if}$. The perpendicular leakage tally, $\mathcal{L}_{kj}$, is divided by the same quantity.

VI. MONTE CARLO CONSTANTS

Storage assignments, geometric data, etc., for the constants for a monte carlo calculation on a system do not change during the course of calculation so that all such quantities are computed only once for each monte carlo system just preceding the first monte carlo time step. The quantities which do change with time are the acceleration factors, A_{ih}^t ; and the quantities dependent on the isotope concentrations in each material, that is, the concentrations themselves which are used in the resonance calculation; the mean free paths, λ_{mi} ; the collision neutron emission numbers, $P_{mi_{el}}$, $P_{mi_{inel}}$, and P_{mi_f} ; and the anisotropic scattering coefficients, $a_{0_{rmi}}$, $a_{1_{rmi}}$, $a_{2_{rmi}}$, and $a_{3_{rmi}}$ for the heavy scatterers which are actually combinations of the heavy scattering isotopes in a material. The equations by which these are calculated are

$$\lambda_{mi} = \left[\sum_{a \text{ in } m} N_{am} c_{ai_T} \times 10^{-24} \right]^{-1}$$

$$P_{mi_{inel}} = \lambda_{mi} \sum' N_{am} (\nu_{inel} \sigma_{inel})_{ai} \times 10^{-24} \quad (55)$$

where the primed sum indicates all isotopes in m having the same value of D , the inelastic spectrum indication. There will be R'_m of the $P_{mi_{inel}}{}_{r'm}$ for group i region m .

$$P_{mi_f} = \lambda_{mi} \sum_{a \text{ in } m} N_{am} (\nu_f \sigma_f)_{ai} \times 10^{-24}$$

$$P_{mi_{el}} = \lambda_{mi} \sum'' N_{am} \sigma_{el_{am}} \times 10^{-24}$$

for heavy isotopes,

$$P_{mi_{el}} = \lambda_{mi} N_{am} \sigma_{el_{am}} \times 10^{-24} \quad (56)$$

for light isotopes.

The doubly primed sum indicates all isotopes in m having atomic weight greater than a_H , an input constant. These are heavy isotopes, moderation by which is assumed to be unimportant except in the resonance range. For scattering

by these isotopes outside the range $I_{H_{1m}} < i < I_{H_{2m}}$ moderation is neglected; within that range a constant atomic weight a_H' is used. For these isotopes the anisotropic scattering coefficients must be averaged:

$$a_{mi} = \left[\sum'' N_{am} \sigma_{ai_{el}} a_{ai} \right] / \sum'' N_{am} \sigma_{ai_{el}} \quad (57)$$

The calculation of a_m is made as follows:

If $a_3 \neq 0$ extrema of $\frac{dP(\mu)}{d\mu}$ lie at

$$\mu_m = \frac{-a_2 \pm \sqrt{a_2^2 - 3a_1 a_3}}{a_3} \quad (58)$$

If

$$a_2^2 - 3a_1 a_3 \geq 0$$

$$-1 \leq \mu_m \leq 1$$

and

$$a_2 + 3a_3 \mu_m < 0, \quad (59)$$

then there is a maximum within the range of μ of interest

and its value is

$$a_m = a_0 + a_1 \mu_m + a_2 \mu_m^2 + a_3 \mu_m^3 \quad (60)$$

If all three equations of (59) are not satisfied for at least one of the solutions of (58), then there is no maximum in the pertinent range and a_m equals the larger of

$$\begin{aligned} a_0 - a_1 + a_2 - a_3 \quad \text{and} \\ a_0 + a_1 + a_2 + a_3 \end{aligned} \quad (61)$$

If $a_3 = 0$ and $a_2 \neq 0$, there is an extremum at

$$\mu_m = -\frac{a_1}{2a_2}$$

and, if the last two of (59) are satisfied the value of a_m is given by (60). If (59) is not satisfied, or if a_2 and a_3 are both zero, then a_m is the larger of (61).

The acceleration factors A_{ih}^t are obtained for the third and subsequent monte carlo step flux tallies as the ratio of the flux in group i , region h in the last monte carlo step to that in the one before

$$A_{ih}^t = \frac{\phi_{ih}^{t-1}}{\phi_{ih}^{t-2}} \quad (62)$$

The albedoes are obtained from the diffusion theory fluxes. Albedoes are non-zero at interfaces between monte carlo systems. In the input to the program, with each boundary (for which an albedo is to be computed) the macroscopic region on the side of it nearest the origin is listed. It is the fluxes in this macroscopic region or the next higher one from which the albedoes are calculated. If the macroscopic region number listed in the input with a boundary is zero, then the program assumes that albedoes are not required for that boundary. The boundaries with which a macroscopic region number is given are those bounding monte carlo systems. In addition to the appropriate macroscopic region number, a number g' which may have the values ± 1 is given in the input. This number is equal to -1 if the boundary is on the origin side of the monte carlo system and is $+1$ if it is on the side of the system farther from the boundary. One further input number given with each boundary is M , a correction factor used to improve the diffusion approximation used in (63).

The equation from which albedoes are calculated is

$$\omega_j = \frac{\phi_{N_k}^{-g'2D_k} \left[\frac{\phi_{N_k,j} - \phi_{N_{k-1},j}}{\Delta r_k} \right]}{\phi_{N_k}^{+g'2D_k} \left[\frac{\phi_{N_k,j} - \phi_{N_{k-1},j}}{\Delta r_k} \right]} M \quad (63)$$

In Equation (63) N_k is the mesh point at the boundary separating region k and region $k + 1$, and D_k and Δr_k are respectively the diffusion coefficients and mesh spacing in region k . In Equation (63) indices referring to the boundary and to the macroscopic energy group have been suppressed. It is to be understood that for each boundary between two systems, an albedo is computed for

each macroscopic group for each of the two systems. In other words the number of albedoes computed preceding a monte carlo on a particular system is J times the number of boundaries in that system for which k values were given. Since the RBU Program begins with a monte carlo calculation performed before the diffusion fluxes are available, it is necessary to input a set of albedoes for the first monte carlo steps.

VII. THE DIFFUSION CALCULATION

As was discussed in the first section of this report, most of the neutron flux and reactivity calculations in RBU are made using the diffusion approximation. The fluxes and other quantities obtained from the monte carlo portion of the program are used to obtain constants for a one space dimensional diffusion calculation. In this, the spatial variable, r , may be either a cartesian coordinate, the radial variable of a set of cylindrical coordinates or the radial variable of a set of spherical coordinates. Its range is divided into a set of discrete points, $R_0 \leq r_n \leq R_N$. The macroscopic region boundaries, as represented in this one dimensional model form a subset R_k of the r_n . Within any macroscopic region, the mesh spacing and the nuclear properties of the system are assumed independent of r .

The second independent variable of the diffusion calculation is the neutron energy, E . The range of this variable, also, is represented by a set of discrete values $E_J \leq E_j \leq E_0$ which correspond to the limits of the macroscopic groups discussed earlier.

In terms of the continuous variables, r and E , the diffusion equation is

$$\begin{aligned}
 & \nabla [D(r,E) \nabla \phi(r,E)] - \Sigma_t(r,E) \phi(r,E) \\
 & + \chi_{in}(r,E) \int_E^{E_0} \Sigma_{in}(r,E') v_{in}(r,E') \phi(r,E') \frac{dE'}{\int_0^{E'} \chi_{in}(r,E'') dE''} \\
 & + \sum_A \int_E^{\min(E/\alpha_A, E_0)} \frac{\Sigma_{sA}(r,E') \phi(r,E') dE'}{(1-\alpha_A)E'} \\
 & = \frac{-\chi_f}{k} \int_{E_J}^{E_0} \Sigma_f(r,E') v_f(r,E') \phi(r,E') dE'
 \end{aligned} \tag{64}$$

The usual approximations namely that χ_{in} is independent of the incident energy except for truncation and renormalization at that value and that elastic scattering is isotropic in the center of mass system have been made in writing (64)

Since the properties of a diffusion calculation on a thermal or intermediate reactor are not very sensitive to the details of the inelastic scattering spectrum and since experimental data does not warrant more detail, the first of these appears perfectly satisfactory. The second approximation also should introduce no detectable error in most calculations; in a sense the use of diffusion theory implies this. Should it become significant in special cases, however, minor changes in the pre-diffusion portion of the program or use of a set of synthetic scatterers can eliminate it.

In terms of the macroscopic energy groups, (64) becomes

$$-\nabla \left[D_j(r) \nabla \phi_j(r) \right] + T_j(r) \phi_j(r) = H_j(r) \quad (65a)$$

$$\left. \begin{aligned} H_j(r) &= \sum_{j'=1}^{i-1} T_{jj'}(r) \phi_{j'}(r) + \chi_j P(r) \\ P(r) &= \frac{1}{\lambda} \sum_{j=1}^J F_j(r) \phi_j(r) \end{aligned} \right\} \quad (65b)$$

The nuclear constants appearing in (65a) and (65b) are defined in the section of this report on Diffusion Constants.

A. THE DIFFERENCE EQUATIONS

With the discrete spatial mesh Equation (65) becomes, on dropping the subscript j

$$-a_n \phi_{n-1} + b_n \phi_n - c_n \phi_{n+1} - d_n = 0 \quad (66)$$

where

$$\left. \begin{aligned} a_n &= (D_{n-}) \frac{r_{n-1/2}^\rho}{\Delta r_{n-}} \\ b_n &= a_n + c_n + (T_{n-}) r_n^\rho \frac{\Delta r_{n-}}{2} + (T_{n+}) r_n^\rho \frac{\Delta r_{n+}}{2} \\ c_n &= (D_{n+}) \frac{r_{n+1/2}^\rho}{\Delta r_{n+}} \\ d_n &= r_n^\rho \frac{\Delta r_{n-}}{2} H_{n-} + r_n^\rho \frac{\Delta r_{n+}}{2} H_{n+} \end{aligned} \right\} \quad (67)$$

$$H_{n-} = \sum_{j=1}^{i-1} T_{n-,jj'} \phi_{nj'} + \chi_j P_{n-}; \quad H_{n+} = \sum_{j=1}^{i-1} T_{n+,jj'} \phi_{nj'} + \chi_j P_{n+} \quad (68)$$

where

$\rho = 0, 1$ or 2 for plane, cylindrical, or spherical geometries respectively

$$\Delta r_{n+} = r_{n+1} - r_n$$

$$\Delta r_{n-} = r_n - r_{n-1}$$

In (66), (67), and (68), minus signs associated with an index, n , indicate values of mesh spacing, power, and nuclear constants appropriate where $r < r_n$ of mesh point n while plus signs indicate those appropriate where $r > r_n$. When r_n does not coincide with a region boundary, R_k , (67) and (68) reduce to

$$\left. \begin{aligned} a_n &= D_n \frac{r_{n-1/2}^\rho}{\Delta r_n} \\ b_n &= a_n + c_n + T_n r_n^\rho \Delta r_n \\ c_n &= D_n \frac{r_{n+1/2}^\rho}{\Delta r_n} \\ d_n &= r_n^\rho \Delta r_n H_n \end{aligned} \right\} \quad (67a)$$

$$H_n = \sum_{j=1}^{i-1} T_{n,jj'} \phi_{nj'} + \chi_j P_n \quad (68a)$$

At the boundaries of the mesh, R_0 and R_N , the equations for $a_{n,j}$, $b_{n,j}$, $c_{n,j}$, and $d_{n,j}$ are modified to agree with the boundary conditions,

$$\begin{aligned} -(1-B_{0,j}) D_{0,j} \frac{\phi_{1,j} - \phi_{0,j}}{\Delta r_{0+}} + B_{0,j} \phi_{0,j} &= 0 \\ (1-B_{N,j}) D_{N,j} \frac{\phi_{N,j} - \phi_{N-1,j}}{\Delta r_{N-}} + B_{N,j} \phi_{N,j} &= 0 \end{aligned} \quad (69)$$

which correspond to the physical boundary conditions

$$\begin{aligned} -[1-B_0(E)] D(R_0, E) \nabla \phi(R_0, E) + B_0(E) \phi(R_0, E) &= 0 \\ [1-B_N(E)] D(R_N, E) \nabla \phi(R_N, E) + B_N(E) \phi(R_N, E) &= 0 \end{aligned} \quad (70)$$

When used in RBU, it is generally true that $R_0 = 0$, $B_0(E) = 0$, $B_N(E) = 1$; the generality of (70) is included in the program to make the use of the diffusion portion without the remainder of RBU convenient.

Equations (69) lead to the following equations for $n = 0$

$$\begin{aligned} a_{0,j} &= 0 \\ b_{0,j} &= -c_{0,j} + B_{0,j} \Delta r_{0+} \\ c_{0,j} &= -(1-B_{0,j}) \\ d_{0,j} &= 0 \end{aligned} \quad (71)$$

and for $n = N$

$$\begin{aligned} a_{N,j} &= (1-B_{N,j}) D_{N,j} \\ b_{N,j} &= -a_{N,j} + B_{N,j} \Delta r_{N-} \\ c_{N,j} &= 0 \\ d_{N,j} &= 0 \end{aligned} \quad (72)$$

B. NUMERICAL METHOD

The spatial integration subject simultaneously to boundary conditions at both ends of the mesh is performed with the use of auxiliary functions $p_{n,j}$ and $q_{n,j}$. Defining these by

$$\phi_{n,j} = p_{n,j} \phi_{n+1,j} + q_{n,j} \quad (73)$$

leads

$$\begin{aligned} p_{n,j} &= \frac{c_{n,j}}{b_{n,j} - a_{n,j} p_{n-1,j}} \\ q_{n,j} &= \frac{d_{n,j} + a_{n,j} q_{n-1,j}}{b_{n,j} - a_{n,j} p_{n-1,j}} \\ p_{-1,j} &= q_{-1,j} = 0 \end{aligned} \quad (74)$$

A process of finding a set of $\phi_{n,j}$ which satisfy Equations (66) and (69) when a set of P_n is known is the following. The $H_{n,1}$ are computed using (68) from χ_1 , and P_n . From these, using (67), (68), (71), and (72) the $a_{n,1}$, $b_{n,1}$, $c_{n,1}$, and $d_{n,1}$ are computed. The $p_{n,1}$ and $q_{n,1}$ may then be computed using Equation (74) successively for $n=0, n=1, \dots, n=N$. Beginning now with $n=N$, the $\phi_{n,1}$ are computed with Equation (73). With the $\phi_{n,1}$, χ_2 , and P_n , the $H_{n,2}$ are now computed and the process above repeated for $j=2$. Continuing in this fashion, all the $\phi_{n,j}$ are found.

The $\phi_{n,j}$ may be used to compute a set of P_n from the discretized version of (65b)

$$P_n = \frac{1}{\mathcal{K}} \sum_{j'=1}^J F_{nj'} \phi_{nj'} \quad (75)$$

where $\mathcal{K}$, the multiplication, is defined by

$$\mathcal{K} \equiv \frac{1}{V} \sum_{n=0}^N \sum_{j'=1}^J \left[F_{n-j'} \Delta r_{n-} + F_{n+j'} \Delta r_{n+} \right] \phi_{n,j} \frac{r_n^\rho}{2}$$

so that

$$\sum_{n=0}^N P_n \Delta V_n = V$$

$$V = \sum_{n=0}^N r_n^{\rho} \left(\frac{\Delta r_{n-}}{2} + \frac{\Delta r_{n+}}{2} \right)$$

$$\Delta r_{0-} \equiv \Delta r_{N+} \equiv P_{0-} \equiv P_{N+} \equiv 0 \quad (76)$$

For values of n in (76) which do not correspond to region boundaries, the terms reduce to $F_n \phi_n r_n^{\rho} \Delta r_n$ and $r_n^{\rho} \Delta r_n$.

The P_n so obtained may be used to repeat the calculation of the ϕ_{jn} and the iterative process continued. Ultimately the values of $\phi_{n,j'}$ and P_n found in this way converge to a consistent solution.

C. ACCELERATION

For reactors in which the multiplications of the second and higher modes is only slightly smaller than that of the first, convergence will be slow; for this reason the procedure described above is modified to improve the rate. The modifications used in RBU are made in the calculation of $H_{n,j}$ in (68) and (68a) and correspond to a combination of the Extrapolated Liebman method and the Aitken δ^2 process. The $\phi_{n,j'}$ in the first term of $H_{n,j}$ appear only for $j' < j$. It is therefore possible to use as was indicated in the preceding description of the process, values obtained in the current iteration, iteration p . The $\phi_{n,j'}$ occurring in the second term (see Equation (75)) appear for all values of j' between 1 and J inclusive some of which are known only for iteration $p-1$. For $j' < j$, however, the values for iteration p are available and it is desirable to use them. Inserting the iteration number in (75) with this modification we have for the $P_n^{(p)}$ from which to compute the $\phi_{n,j+1}^{(p)}$

$$P_{n(j)}^{(p)} = \frac{1}{\mathcal{E}_{(j)}} \left[\sum_{j'=1}^j F_{nj'} \phi_{n,j'}^{(p)} + \sum_{j'=j+1}^J F_{nj'} \phi_{n,j'}^{(p-1)} \right] \quad (77)$$

The group subscript, j , in (77) is placed in parenthesis to indicate that while P_n and k are not strictly a function of j , the method used here for their evaluation, makes the values vary according to the group being worked on at any stage of the calculation. The value of k appearing in (77) is defined in (76) as before but it must now be re-evaluated at each group.

There is one further modification to be made to obtain the final form of (75). This is to use for $P_{n(0)}^{(p+1)}$ a value which is extrapolated beyond that given by (77) in accordance with our information about $P_{n(0)}^{(p)}$.

$$P_{n(0)}^{(p+1)} = P_{n(j)}^{(p)} + \omega \left(P_{n(j)}^{(p)} - P_{n(0)}^{(p)} \right) \quad (78)$$

where ω is an acceleration factor supplied as input and $P_{n(0)}^{(p)}$ is the source from which the fluxes of the first group for iteration p are computed. Equation (77) implies a complete re-evaluation of P_n for each group. Actually, this is not necessary since only the changes in k and P_n resulting from the difference $\phi_{n,j}^{(p)} - \phi_{n,j}^{(p-1)}$ need be considered. Thus,

$$P_{n(j)}^{(p)} = \frac{1}{k_{(j)}} \left[k_{(j-1)} P_{n(j-1)} + F_{n,j} \left(\phi_{n,j}^{(p)} - \phi_{n,j}^{(p-1)} \right) \right]$$

$$k_{(j)} = k_{(j)} + \frac{1}{v} \sum_n \left(\phi_{n,j}^{(p)} - \phi_{n,j}^{(p-1)} \right) \left(F_{n-j} \Delta r_{n-} + F_{n+j} \Delta r_{n+} \right) \frac{r_n^0}{2} \quad (79)$$

In solving equations of the form $F(\alpha) = \alpha$ by an iterative procedure of the type

$$\alpha_{p+1} = F(\alpha_p) \quad (80)$$

it is possible to estimate the value of the root from the values of three successive iterates by Aitken's δ^2 process. The error in the p^{th} iterate is

$$\alpha - \alpha_p = F(\alpha) - F(\alpha_{p-1}) \quad (81)$$

which may be expanded in a Taylor's series about α :

$$\alpha - \alpha_p = (\alpha - \alpha_{p-1}) F'(\alpha) + \dots \quad (82)$$

Provided either that

$$\alpha - \alpha_p < < 1 \quad \text{or} \quad F''(\alpha) < < F'(\alpha) \quad (83)$$

the higher order terms may be dropped, and α can be determined from the values of three successive α_p :

$$\frac{\alpha - \alpha_p}{\alpha - \alpha_{p-1}} = \frac{\alpha - \alpha_{p-1}}{\alpha - \alpha_{p-2}}$$

$$\alpha \approx \alpha_p + \frac{(\alpha_p - \alpha_{p-1})^2}{\alpha_p - 2\alpha_{p-1} + \alpha_{p-2}} \quad (84)$$

It is clear that the process for getting P_n described above can be written as a set of coupled equations of the form (81). Equation (82) then takes the form

$$\alpha_n - \alpha_n^{(p)} = \sum_{n'=1}^N \left(\alpha_{n'} - \alpha_{n'}^{(p)} \right) \frac{\partial F_n(\alpha_1^{(p)}, \alpha_2^{(p)}, \dots, \alpha_N^{(p)})}{\partial \alpha_{n'}} \quad (85)$$

On the assumption that $\frac{\partial F_n}{\partial \alpha_{n'}}$ is small for $n' \neq n$, (84) appears to be a valid method to estimate P_n . For this reason after each set of three iterations carried out as described in (79) the set of P_n used in (68a) for the next iteration is obtained from (84) rather than from (79). Equation (84), however, involving, as it does, a ratio of differences, may become inaccurate when the successive α_p differ only in a few of the least significant digits. For this reason, when the precision of the differences involved becomes less than fifteen bits for a particular mesh point, the program ceases to use the Aitken δ^2 process for that mesh point.

D. SPECIFIC NUMERICAL PROCEDURE

In the following paragraphs, the numerical process of manipulating the P_n and k is outlined in detail. For clarity the discussion begins at a point in the diffusion calculation during the p^{th} iteration when

fluxes for group $j-1$ have been calculated and the multiplication and source corrected to give a value of $k_{(j-1)}^{(p)}$ and a set of $p_{n(j-1)}^{(p)}$ for $n = 0^+, 1, 2 \dots N_1^-, N_1^+ \dots N^-$. Using the $p_{n(j-1)}^{(p)}$, the fluxes for group j , $\phi_{n,j}^{(p)}$, are found by means of Equations (67) through (74). Then

$$k_{(j)}^{(p)} = k_{(j-1)}^{(p)} + \frac{1}{V} \sum_n \Delta V_n F_{nj} \left(\phi_{n,j}^{(p)} - \phi_{n,j}^{(p-1)} \right) \quad (86)$$

where it is understood that

$$\Delta V_n F_{nj} = \frac{r_n^0}{2} \left[F_{n^-j} \Delta r_{n^-} + F_{n^+j} \Delta r_{n^+} \right] \quad (87)$$

if n corresponds to a region boundary,

and is simply $r_n^0 F_{nj} \Delta r_n$ if n does not correspond to a region boundary.

Similarly,

$$p_{n(j)}^{(p)} = \frac{1}{k_{(j)}^{(p)}} \left[k_{(j-1)}^{(p)} p_{n(j-1)}^{(p)} + F_{nj} \left(\phi_{n,j}^{(p)} - \phi_{n,j}^{(p-1)} \right) \right] \quad (88)$$

This process is continued for each group until the $p_{n(J)}^p$ and $k_{(J)}^p$ have been found. If

$$\left| k_{(J)}^{(p)} - k_{(J)}^{(p-1)} \right| > \epsilon_3 \text{ or if, for any } n, \frac{\left| p_{n(J)}^{(p)} - p_{n(J)}^{(p-1)} \right|}{p_{n(J)}^p} > \epsilon_4 \quad (89)$$

another iteration is to be carried out. If two successive iterates obtained by (88) and a third obtained just previously are not available, then the next iteration is similar to that just described but, before beginning it, the latest sources are accelerated

$$p_{n(0)}^{(p+1)} = p_{n(J)}^{(p)} + \omega \left(p_{n(J)}^{(p)} - p_{n(0)}^{(p)} \right)$$

$$k_{(0)}^{(p+1)} = k_{(J)}^{(p)} \quad (90)$$

and the $\phi_{n,j}^{(p)}$ are replaced by

$$\phi_{n,j}^{(p)} + \omega \left(\phi_{n,j}^{(p)} - \frac{\phi_{n,j}^{(p)} - \phi_{n,j}^{(p-1)}}{\phi_{n,j}^{(p)} - \phi_{n,j}^{(p-1)}} \phi_{n,j}^{(p-1)} \right) \rightarrow \phi_{n,j}^{(p)} \quad (91)$$

With the $P_{n(0)}^{(p+1)}$ a set of $\phi_{n,1}^{(p+1)}$ are found. Equations (86) and (88) may then be solved and the process continued.

If three sets of $P_{n(0)}$ are available, the last two of which were obtained from (88), the Aitken δ^2 process is used to recompute the $P_{n(0)}^{(p+1)}$. In this case $P_{n(0)}^{(p+1)}$ is computed by (90) as before but

$$P_n^{(p+1)} = P_{n(0)}^{(p+1)} - \frac{\left(P_{n(0)}^{(p+1)} - P_{n(0)}^{(p)} \right)^2}{P_{n(0)}^{(p+1)} - 2 P_{n(0)}^{(p)} + P_{n(0)}^{(p-1)}} \quad (92)$$

is computed for those n for which the differences in the numerator and denominator of (93) have fifteen or more significant bits. For values of n for which this is not the case $P_n^{(p+1')} = P_{n(0)}^{(p+1)}$ as obtained from (90). Then the $P_{n(0)}^{(p+1)}$ are replaced by

$$V = \frac{P_n^{(p+1')}}{\sum_{n'} \Delta V_{n'} P_{n'}^{(p+1')}} \rightarrow P_{n(0)}^{(p+1)} \quad (93)$$

Unfortunately, this set of sources bears no simple relationship to any available set of fluxes so that the groupwise correction procedure of (86) and (88) may not be used. Instead the same set of sources, that computed in (93), is used to calculate the fluxes $\phi_{n,j}^{(p+1)}$ for all j . When the $\phi_{n,j}^{(p+1)}$ have been computed, a new multiplication and set of sources is computed from

$$\phi_0^{(p+2)} = \frac{1}{V} \sum_n \Delta V_n \sum_j F_{nj} \phi_{n,j}^{(p+1)} \quad (94)$$

and

$$P_{n(0)}^{(p+2)} = \frac{1}{\phi_{(1)}^{(p+2)}} \sum_j F_{nj} \phi_{n,j}^{(p+1)}$$

Iteration $p+2$ then proceeds by the use of (86) and (88).

At any time step other than the first, the program begins with a set of $\phi_{n,j}$, a set of $P_{n(J)}$, and a $k_{(J)}$ which were the result of the last iteration performed on the previous time step. These are identified as the $\phi_{n,j}^{(0)}$, $P_{n(0)}^{(1)}$, and $k_{(0)}^{(1)}$ for the present time step and the procedure outlined above can then be followed

For the first time step, the fluxes, power, and multiplication are not available. A set of $\phi_{n,j}$ is generated as follows

$$\phi_{n,j} = 0, \quad j \neq J$$

$$\phi_{n,J} = \frac{V}{\sum_n \Delta V_n F_{nJ}}, \quad n = 0, 1, \dots, N \quad (95)$$

These are identified as the $\phi_{n,j}^{(0)}$; the $P_{n(0)}^{(1)}$ are

$$P_{n(0)}^{(1)} = \frac{V}{\sum_n \Delta V_n F_{nJ}} F_{nJ} \quad (96)$$

and the $k_{(0)}^{(1)}$ is unity.

VIII. THE DIFFUSION CONSTANTS

The nuclear constants of Equation (65) are, in general, weighted averages of the microscopic group and region constants used in the monte carlo portion of the program with the monte carlo fluxes used as the weight functions. The exceptions to this are the diffusion coefficients D_{jk} , the perpendicular leakage cross section, and, in addition, all constants whose equivalent, in the monte carlo portion are computed from Breit Wigner resonance function.

For those macroscopic groups and regions not encompassing a resonance range in any of its microscopic groups and regions, a typical macroscopic group average cross section is

$$\Sigma_{jmp} = \sum_{a \text{ in } m} N_{a_m} \sigma_{ajmp} \times 10^{-24} \quad (97)$$

where

$$\sigma_{ajmp} = \left[\sum_{i \text{ in } j} \sigma_{aip} \phi_{im} \right] / \sum_{i \text{ in } j} \phi_{im}$$

$$\phi_{im} = \sum_{f \text{ containing } m} \phi_{if} \quad (98)$$

The subscript a refers to a particular isotope, p specifies a cross section type and m is the index of the material contained in region h, a region of region set f.

The average over the microscopic region sets in a macroscopic region is

$$\Sigma_{jkp} = \left[\sum_{m \text{ in } k} \Sigma_{jmp} \phi_{jm} \right] / \sum_{m \text{ in } k} \phi_{jm} \quad (99)$$

where

$$\phi_{jm} = \sum_{i \text{ in } j} \phi_{im} \quad (98a)$$

The calculations corresponding to (98) and (98a) are made after each monte carlo step while those corresponding to (97) and (99) are made after each burnup step and each monte carlo step.

The calculations corresponding to (98) are specifically

$$t_{ajm} = \left[\sum_{i \text{ in } j} \sigma_{ait} \phi_{im} / \sum_{i \text{ in } j} \phi_{im} \right]^{-t_{ajjm}} \quad (100)$$

$$t_{ajj'm} = \left\{ \begin{aligned} &= P_{j'} \left[\sum_{i' \text{ in } j'} \chi_{aji'} (\sigma_{in' in})_{ai'} \phi_{i'm} (E_{j-1} - E_j)^{-1} \right. \\ &+ \frac{2}{1-\alpha_a} \sum_{\substack{i' \text{ in } j' \\ i' > i(\alpha_j)}} \sigma_{ai's} \frac{\phi_{i'm}}{(E_{i'} + E_{i'-1})} \\ &+ \epsilon(jj'\alpha) \frac{2}{1-\alpha_2} \sigma_{a,i(\alpha_j),s} \frac{\phi_{i(\alpha_j)}}{E_{i(\alpha_j)} + \frac{E_{j-1}}{\alpha}} \frac{\frac{E_{j-1}}{\alpha} - E_{i(\alpha_j)}}{E_{i(\alpha_j)-1} - E_{i(\alpha_j)}} \left. \right] \\ &= 0, \end{aligned} \right. \quad \begin{aligned} &\text{if } j \geq j' \\ &\text{if } j < j' \end{aligned} \quad (101)$$

In Equation (101) $i(\alpha, j)$ is the group such that

$$E_{i(\alpha_j)} < \frac{E_{j-1}}{\alpha} \leq E_{i(\alpha_j)-1}$$

while

$$\epsilon(jj'\alpha) = 0 \quad \text{if } \frac{E_{j-1}}{\alpha} \geq E_{j'-1}$$

$$= 1 \quad \text{if } E_{j'} < \frac{E_{j-1}}{\alpha} < E_{j'-1} \quad (102)$$

and

$$P_{j'} = (E_{j'-1} - E_{j'}) / \sum_{i' \text{ in } j'} \phi_{i'm} \quad (103)$$

The term $\chi_{aji'}$ is obtained from the evaporation model constants or inelastic spectrum table $[P_n, (v)_n^2]$

$$\chi_{aji'} = \left(P_{n_1(j)} - P_{n_2(j)} \right) / P_{n_3(i')} \quad (104)$$

where $P_{n_1(j)}$ is the entry in the table such that

$$(v^2)_{n_1(j)+1} > 1.916 (E_{i'} - E_j) > (v^2)_{n_1(j)}$$

$P_{n_2(j)}$ is the entry in the table such that

$$(v^2)_{n_2(i')+1} > 1.916 (E_{i'} - E_{j-1}) > (v^2)_{n_2(j)}$$

and $P_{n_3(i')}$ is the entry such that

$$(v^2)_{n_3(i')+1} > 1.916 E_{i'} > (v^2)_{n_3(i')}$$

(105)

For isotopes using the evaporation model

$$\chi_{aji'} = \frac{e^{-E_j/T} (E_{j-1} + T) - e^{-E_{j-1}/T} (E_{j-1} + T)}{T - e^{-E_{i'}/T} (E_{i'} + T)} \quad (106)$$

where

$$T = 1.384D \sqrt{E_i}$$

The fission coefficient is

$$f_{ajm} = \frac{(E_{j-1} - E_i)}{\sum_{i \text{ in } j} \phi_{im}} \sum_{i \text{ in } j} (\sigma_f v_f)_{ai} \phi_{im} \quad (107)$$

while the fission spectrum coefficient χ_f is obtained from the monte carlo fission spectrum data (P_n, V_n)

$$\chi_{fj} = \left[P_{n(j-1)} - P_{n(j)} + \frac{E_{j-1} - 0.5224V_{n(j-1)}^2}{0.5221 (V_{n(j-1)+1}^2 - V_{n(j-1)}^2)} \frac{(P_{n(j-1)+1} - P_{n(j-1)})}{(E_{j-1} - E_j)} \right] \quad (108)$$

where $n(j)$ and $n(j-1)$ are defined by

$$0.5221 V_{n(j-1)}^2 \leq E_{j-1} < 0.5221 V_{n(j-1)+1}^2$$

$$0.5221 V_{n(j)}^2 \leq E_j \leq 0.5221 V_{n(j)+1}^2 \quad (109)$$

While preparing the diffusion constants, an additional constant Σ_f is computed by equations identical to that for f_{ajm} and F_{jk} except for the replacement of $\sigma_f \nu_f$ by γ_f . This is used in the calculation of Burnup Constants to obtain the average value of ν

The diffusion coefficient is not computed individually for each isotope and material but is obtained for each macroscopic group and region directly from monte carlo tallies. Therefore D_{jk} does not change as a direct result of a burnup step but is modified only after a monte carlo calculation.

$$D_{jk} = \frac{L_{kj}}{(n \nabla^2 \phi)_{kj}} \quad (110)$$

For those materials and groups involving resonances, the contributions to the nuclear constants t_{ajm} , $t_{ajj'm}$, f_{ajm} are obtained by using the quantities in (111) for the values σ_{ait} , σ_{ais} , σ_{aic} , and $(\sigma_f \nu_f)_{ai}$ in (100), (101), and (107) in groups in which a has unresolved resonances.

$$\begin{aligned} (\tilde{\sigma}_f \nu_f)_{ai} &= (\Sigma_f \phi)_{ajm} \nu_{far} / \sum_{i \text{ in } j} \phi_{im} N_{am} \\ \tilde{\sigma}_{aic} &= (\Sigma_c \phi)_{ajm} / \sum_{i \text{ in } j} \phi_{im} N_{am} \\ \tilde{\sigma}_{ais} &= (\Sigma_s \phi)_{ajm} / \sum_{i \text{ in } j} \phi_{im} N_{am} \\ \tilde{\sigma}_{ait} &= \tilde{\sigma}_{fai} + \tilde{\sigma}_{aic} + \tilde{\sigma}_{ais} \end{aligned} \quad (111)$$

Note that the quantities on the left of (111) will actually be independent of i within a given macroscopic group j since the monte carlo unresolved resonances tallies on the right are only made by macroscopic group. The term ν_{far} is the value given for unresolved resonance groups in a. These quantities are computed just after a monte carlo step using the N_{am} which were used in the monte carlo.

The microscopic diffusion calculation constants described above are computed after each monte carlo step. Macroscopic values are obtained from

Equation (97) and (99) after each burnup or monte carlo step. For example,

$$T_{jm} = \sum_{a \text{ in } m} N_{am} t_{jm} \times 10^{-24}$$

$$T_{jk} = \sum_{m \text{ in } k} T_{jm} \phi_{jm} / \sum_{m \text{ in } k} \phi_{jm}$$

To the T_{kj} thus obtained must be added the quantity

$$\mathcal{L}_{kj} / \sum_{i \text{ in } j} \sum_{f \text{ in } k} \phi_{if}$$

to account for the perpendicular leakage usually represented by the pseudo cross section B^2D .

IX. ITERATION ON THE REACTIVITY

The input contains a list of microscopic region set numbers in a sequential order which represent the reactivity regulating system of the reactor. Reactivity is altered by changing the material in a region set in this sequence from one to another of four materials listed in order of increasing contribution to reactivity with the region set number in the sequence. When the required adjustment of reactivity is greater than that which can be obtained by use of one of the extreme materials for the region set, the program passes on to the next region set in the sequence and begins to adjust this.

Explicitly, the control regions sets are those with microscopic region set numbers included in the input list:

$$c_1, c_2, c_3, \dots, c_\ell, \dots, c_L$$

Associated with each index c_ℓ in this list are four material indices $m_{c_{\ell_1}}$, $m_{c_{\ell_2}}$, $m_{c_{\ell_3}}$, $m_{c_{\ell_4}}$. The material actually in each region set, as identified by the material indices stored in the normal places for the regions of the set, is one of these four. A number k indicates which of the L control region sets is currently modifiable for adjustment of criticality. On completion of a diffusion calculation, the program determines if the difference between the multiplication and unity is within specified tolerance limits

$$|k - 1| \leq \epsilon_5 \quad (112)$$

If it is, then no adjustment of control need be made and the program proceeds to the next portion of the calculation, normally a burnup step.

If (112) is not satisfied, then a change is made in the material contents of the regions of region set c_ℓ . If $k < 1$ then this material is changed from that presently in them to the next one in the sequence $m_{c_{\ell_1}}$, $m_{c_{\ell_2}}$, $m_{c_{\ell_3}}$, $m_{c_{\ell_4}}$.

If the current material is already $m_{c_{\ell_4}}$, then ℓ is increased by one and the change is made in the material in the regions of the region set corresponding to the new value of ℓ . If the increase in ℓ makes it greater than L , the

program stops since this indicates that the reactivity life has been exhausted.

Similarly if (112) is not satisfied and $\ell > 1$ the change made in the material in the regions of region set c_ℓ is to the previous one in the sequence of materials available for this set. If the current material is already $m_{c_{\ell_1}}$, then ℓ is decreased by one and the change is made in the material in the regions of the region set corresponding to the new value of ℓ . If the change in ℓ makes it less than unity, the program stops since this indicates insufficient reactivity control.

Having changed the appropriate material, the program makes the appropriate corrections in those portions of the burnup and diffusion constants normally computed after a monte carlo, then in the constants of the diffusion calculation for the macroscopic region in question and returns to the diffusion calculation. The corrections in cross sections are made by recomputing the particular values pertaining to the m , f , and k of Equations (97), (98), (99), (100), (101), (107), and (123).

X. THE BURNUP CALCULATION

The change in concentration of an isotope in RBU is governed by the differential equation

$$\frac{\partial N_{am}}{\partial t} = \sum_{a'} N_{a'm} \left(\sum_j \sigma_{a' \rightarrow a, j, k, m} \phi_{jk} + \lambda_{a' \rightarrow a} \right) - N_{am} \left(\sum_j \sigma_{a, j, k, m} \phi_{jk} + \lambda_a \right) \quad (113)$$

N_{am} is the atomic concentration of isotope a in material m ; $\sigma_{a' \rightarrow a, j, k, m}$ is the microscopic cross section of isotope a' in macroscopic energy group j and material m for reactions producing isotope a obtained by flux weighted averaging over the microscopic region sets containing material m ; ϕ_{jk} is the neutron flux density in macroscopic group j averaged over region k ; $\lambda_{a' \rightarrow a}$ is the radioactive decay constant of isotope a' for disintegrations producing isotope a ; $\sigma_{a, j, k, m}$ is the cross section of isotope a in group j and material m for reactions which destroy isotope a ; and λ_a is the total radioactive decay constant of isotope a . The "cross sections" in (113) contain factors to account for the energy span of group j and for the reactor power level. Cross sections and fluxes in (113) are obtained from microscopic group cross sections by a procedure similar to that discussed in the previous section on Diffusion Constants. The calculation of these and the fluxes will be described in the section on Burnup Constants; in this section the discussion is limited to the solution of the sets of equations represented for each of the isotopes present in a material m . For this purpose (113) may be rewritten

$$\dot{N}_{am} = \sum_{a'} N_{a'm} G_{a'} \quad (\text{all } a' \text{ in } m; \text{ all } m \text{ in the problem}) \quad (114)$$

Equation (114) is solved to give the values of the N_{am} at discrete points in time, the time interval, in general, being different for each material. The time interval is expressed as the product $N_{BU} \Delta t$ where Δt is the basic time step for the problem - the interval during which all macroscopic fluxes are assumed constant. Thus, a diffusion calculation is made at each interval Δt . Following a diffusion step, a burnup calculation is done for some material and, of course, it is the changes in concentrations resulting from a burnup step (or the changes in macroscopic region cross sections resulting from a monte carlo) that causes the results of two successive diffusion calculations

to differ. For this reason at least one of the N_{BU} must be unity and, no N_{BU} can be less than unity. The solution of (114)^m is carried out by means of a predictor-corrector method due to Adams so that, after the first two burnup steps on a material, an estimate of the precision is available. This estimate for each isotope in a region is compared with a pair of tolerance limits, ϵ_1 and ϵ_2 to determine whether N_{BU_m} should be increased or decreased.

A. THE PREDICTOR-CORRECTOR METHOD

Calculations of the concentrations are made using estimates of the first through fourth derivatives obtained from the differences of values of the previous first derivatives. Thus predictions are made with

$$p N^{\rho} = N^{\rho-1} + N_{BU} \Delta t \sum_{i=0}^3 \alpha_i (\nabla^i N^{\rho-1})$$

$$\alpha_0 = 1, \alpha_1 = \frac{1}{2}, \alpha_2 = \frac{5}{12}, \alpha_3 = \frac{3}{8} \quad (115)$$

using the backward differences

$$\nabla^0 y^{\rho} = y^{\rho}$$

$$\nabla^1 y^{\rho} = y^{\rho} - y^{\rho-1}$$

$$\nabla^2 y^{\rho} = \nabla^1 y^{\rho} - \nabla^1 y^{\rho-1} = y^{\rho} - 2y^{\rho-1} + y^{\rho-2}$$

$$\nabla^3 y^{\rho} = \nabla^2 y^{\rho} - \nabla^2 y^{\rho-1} = y^{\rho} - 3y^{\rho-1} + 3y^{\rho-2} - y^{\rho-3} \quad (116)$$

In (115)* the superscript ρ indicates the time at which the concentrations and their rates of change apply. The term $p N^{\rho}$ is the concentration at time t_{ρ} estimated from data available at time $t_{\rho-1}$. The data available at this time is the concentration $N^{\rho-1}$, the rate of change at $t_{\rho-1}$, $\nabla^1 N^{\rho-1}$; and the higher order differences of N , $\nabla^i N^{\rho-1}$ ($i=1,2,3$) which yield information of the second through fourth derivatives of N in recent time steps. The zeroth order difference, $\nabla^0 N^{\rho-1} = N^{\rho-1}$ is obtained from (114) using the fluxes and (predicted) concentrations at $t_{\rho-1}$. The fluxes used for this purpose depend, of course, on the properties of all regions in addition to those containing material m ; the

* Equation (115) as well as Equations (117) and (120) are derived in Appendix E

implications of this will become more apparent in the subsequent discussion.

When the rate of change of concentration at t_p is available, another estimate of N^p may be made; this is termed the corrector:

$${}_c N^p = N^{p-1} + N_{BU} \Delta t \sum_{i=0}^3 \beta_i (\nabla^i N^p)$$

$$\beta_0 = 1, \beta_1 = -\frac{1}{2}, \beta_2 = -\frac{1}{12}, \beta_3 = -\frac{1}{24} \quad (117)$$

The agreement between ${}_p N^p$ and ${}_c N^p$ is a measure of the extent to which the time interval $N_{BU} \Delta t$ is satisfactory. If the two disagree excessively this is an indication either that changes in concentration of other isotopes in the same material or higher terms in the expansion of the rate of depletion of the isotope in question lead to a requirement for a shorter time step or that indirect effects of changes in other materials are causing errors. These indirect effects may be understood as follows.

Consider two materials A and B and suppose that at the time t the changes in concentration of one of the isotopes in material B begin to produce rapid changes in the fluxes in regions containing materials A and B. If the predictor in material A is computed from fluxes obtained before this rapid change and the corrector is computed from fluxes obtained after the calculation of new concentrations in material B, an excessive disagreement between the predicted and corrected concentrations of isotopes in material A may be expected.

This will cause the program to decrease N_{BU_A} . If $N_{BU_A} > N_{BU_B}$ this course of action will lead to an improvement in the accuracy of calculation in material A because the changes in fluxes will be more frequently taken into account. If $N_{BU_A} \leq N_{BU_B}$, decreasing N_{BU_A} cannot be expected to improve the accuracy in material A. The same changes which caused disagreement in A, will presumably cause disagreement in B, however, so that N_{BU_B} will be decreased leading to higher accuracy in both materials.

After the effects of the decrease in N_{BU_B} have been felt, the program may find it possible to restore N_{BU_A} to its former value.

B. CHANGING THE TIME INTERVAL

The changes in the N_{BU} are controlled through the comparison of relative errors in predicted and corrected concentrations with two tolerance limits, ϵ_1 and ϵ_2 . If

$$\left| \frac{N_p - N_c}{N_a} \right| < \epsilon_2 \quad (118)$$

for all isotopes in material m then N_{BU_m} will be increased by a factor of two for the next prediction. If

$$\left| \frac{N_p - N_c}{N_a} \right| > \epsilon_1 \quad (119)$$

for any isotope in material m then N_{BU_m} will be decreased by a factor of 2 for the next prediction.

When an N_{BU} is decreased, backward differences, ∇^i , corresponding to the new time interval are required for the next prediction. The philosophy followed here is that ϵ_1 is sufficiently small that when a relative error greater than ϵ_1 is detected at time t , the data available will still be satisfactory for prediction to the time point at $t + N_{BU_m} \Delta t$. (In this expression N_{BU_m} is the new value.) With this point of view, the rates of change of concentration at recent intermediate points may be found using Newton's interpolation formulas. If $\dot{N}(t)$ is the latest value just computed, $N_{BU} \Delta t$ the new time interval and subscripts on the ∇^i indicate whether they are associated with the old or new interval

$$\begin{aligned} \dot{N}(t - 2N_{BU} \Delta t) &= \dot{N}(t) - \nabla_{old}^1 \dot{N}(t) \\ \dot{N}(t - N_{BU} \Delta t) &= \sum_{i=0}^3 \gamma_i \left(\nabla_{old}^i \dot{N}(t) \right) \\ \dot{N}(t - 3N_{BU} \Delta t) &= \sum_{i=0}^3 \gamma_i' \left(\nabla_{old}^i \dot{N}(t) \right) \end{aligned} \quad (120)$$

$$\gamma_0=1, \gamma_1=-\frac{1}{2}, \gamma_2=-\frac{1}{8}, \gamma_3=-\frac{1}{16}$$

$$\gamma'_0=1, \gamma'_1=-\frac{3}{2}, \gamma'_2=-\frac{3}{8}, \gamma'_3=-\frac{1}{16} \quad (120)$$

$$\nabla^0 \dot{N}(t) = \dot{N}(t)$$

$$\nabla_{\text{new}}^1 \dot{N}(t) = \dot{N}(t) - \dot{N}(t - N_{\text{BU}} \Delta t)$$

$$\nabla_{\text{new}}^2 \dot{N}(t) = \dot{N}(t) - 2\dot{N}(t - N_{\text{BU}} \Delta t) + \dot{N}(t - 2N_{\text{BU}} \Delta t)$$

$$\nabla_{\text{new}}^3 \dot{N}(t) = \dot{N}(t) - 3\dot{N}(t - N_{\text{BU}} \Delta t) + 3\dot{N}(t - 2N_{\text{BU}} \Delta t) - \dot{N}(t - 3N_{\text{BU}} \Delta t) \quad (121)$$

When an N_{BU} is to be increased the ∇_{new}^i are computed for the larger time interval. If the terms $p \dot{N}(t)$ and $c \dot{N}(t)$ are the values of concentration which agreed sufficiently well to indicate the possibility of increasing the time interval to the new value $N_{\text{BU}} \Delta t$, then the quantities available are

$$\begin{aligned} \dot{N}(t) &\equiv \nabla_{\text{old}}^0 \dot{N}(t); \dot{N}\left(t - \frac{1}{2} N_{\text{BU}} \Delta t\right) \equiv \nabla_{\text{old}}^0 \dot{N}\left(t - \frac{1}{2} N_{\text{BU}} \Delta t\right); \\ \nabla_{\text{old}}^1 \left(t - \frac{1}{2} N_{\text{BU}} \Delta t\right); \nabla_{\text{old}}^2 \left(t - \frac{1}{2} N_{\text{BU}} \Delta t\right); \nabla_{\text{old}}^3 \left(t - \frac{1}{2} N_{\text{BU}} \Delta t\right) \end{aligned} \quad (122)$$

From these $\dot{N}(t - N_{\text{BU}} \Delta t)$ and $\dot{N}(t - 2N_{\text{BU}} \Delta t)$ may be found leading to values $\nabla_{\text{new}}^0 \dot{N}(t)$, $\nabla_{\text{new}}^1 \dot{N}(t)$, and $\nabla_{\text{new}}^2 \dot{N}(t)$ by equations similar to (121).

There are a number of complications modifying the procedures described so far in this section. These arise primarily from the fact that the set of ∇^i is not always complete. The modifications need not be discussed in detail here, essentially the program uses what information is available, terminating the series in (116), (117), and (120) before the ∇^3 term if fewer ∇^i are available.

A second modification arises from the necessity that no N_{BU_m} be less than unity and that at least one N_{BU_m} be equal to unity. After each burnup in which the changes in the N_{BU_m} described above have been

made for each of the materials for which the relative difference between predicted and corrected values dictates a change, all N_{BU} are examined to determine if these conditions hold. If any N_{BU_m} is one half, the basic time step, Δt , is decreased by a factor of two and all N_{BU_m} multiplied by two. Since this does not affect any values of $N_{BU_m} \Delta t$, it is not necessary to change any of the ∇_{am}^i . Similarly if all N_{BU_m} are greater than one, Δt is doubled and the N_{BU_m} are halved. Because of the fact that increasing a particular N_{BU_m} may result in a change in the basic time step, Δt , affecting the points in time at which it is possible to do burnup calculations on other materials, an increase in an N_{BU_m} can only be made at certain times. Synchronization of all materials is assured by requiring that the time at which the change in N_{BU_m} is to be made is an integral multiple of the new time step $2N_{BU_m} \Delta t$.

XI. BURNUP CONSTANTS

The evaluation of constants for the burnup calculation proceeds in two steps as does that of the diffusion constants. Following a monte carlo calculation, the effective cross sections for macroscopic groups per unit concentration in each material and per unit flux density in diffusion region k containing that material

$$\sigma_{a' \rightarrow a, j, k, m} = 2.72 \times 10^{-6} (E_{j+1} - E_j) P \left[\sum_{i \text{ in } j} \sigma_{a' \rightarrow a, i} \phi_{imk} \right] / \sum_{i \text{ in } j} \phi_{imk} \quad (123)$$

where

$$\phi_{imk} = \sum_{f \text{ containing } m} \phi_{if}$$

Equation (123) contains several factors included for convenience which makes the quantity on the left not strictly a cross section. P is the input value of the operating power density in kilowatts per cubic centimeter. The constant 2.72×10^{-6} includes a factor 10^{-24} to convert barns to square centimeters, a factor to convert power density to density of fissions per second, and a factor to convert time from days to seconds.* To obtain this constant the energy released per fission was assumed to be 198 mev.

To obtain the rate of production of isotope a in atoms per cm^3 per day per unit concentration of isotope a' (in material m) by reactions represented by $\sigma_{a' \rightarrow a}$ it is necessary to multiply by the diffusion fluxes integrated over region k.

$$\dot{N}_{am} = N_{am} \sum_j \sigma_{a' \rightarrow a, jkm} \phi_{jk} + \text{terms due to other reactions}$$

where

$$\phi_{jk} = \frac{\Delta x_k}{V_k} \left[\frac{1}{2} r_{N_{k-1}}^{\rho} \phi_{N_{k-1}} + \sum_{n=N_{k-1}+1}^{N_k-1} r_n^{\rho} \phi_{jn} + \frac{1}{2} r_{N_k}^{\rho} \phi_{jN_k} \right] \nu \quad (124)$$

* Although the unit used for time in the monte carlo portion of RBU is micro-seconds, the burnup portion uses days.

$$V_k = \Delta r_k \left[\frac{1}{2} r_{N_{k-1}}^0 + \sum_{n=N_{k-1}+1}^{N_k-1} r_n^0 + \frac{1}{2} r_{N_k}^0 \right] \quad (125)$$

The factor ν in (124) is the average number of neutrons per fission arising from the fact that the ϕ_{nj} are normalized to one source neutron per unit volume

$$\nu = \frac{\sum_k \sum_j F_{kj} \phi_{kj}}{\sum_k \sum_j \Sigma_{f_{kj}} \phi_{kj}} \quad (126)$$

The appropriate cross sections to be used in Equation (123) are determined from the table of direct descendants and modes of production prepared by the cross section preparation routine from the basic library. Cross sections which may be included in (123) are σ_c , $\sigma_{n,2n}$ and σ_f .

As indicated in Equation (113), another term in (124) involves the total absorption cross section for isotope a . This is $\sigma_c + \sigma_{n,2n} + \sigma_f$. Finally (113) involves the radioactive decay terms $\lambda_{a \rightarrow a}$ and λ_a which are used exactly as they appear in the list of properties of the isotopes and are in reciprocal days. The appropriate identification between λ_a , $\lambda_{a \rightarrow a}$ and a is made through the table of direct descendants and modes.

For isotopes having random resonances in a group i within group j , the $\sigma_{a \rightarrow a, i}$ in (123) are not available from basic cross section data. The $\sigma_{a \rightarrow a, j}$ instead are obtained as in Equation (111) directly from the monte carlo tallies and replaces the factor

$$\sum_i c_i \phi_i / \sum_i \phi_i$$

in (123)

XII. CROSS SECTION PREPARATION ROUTINE

The purpose of the cross section preparation routine is to assemble data on isotope properties from a basic library of isotopic data and a relatively small amount of problem input. The program selects the necessary data from the library, organizes it into cross sections corresponding to the energy group structure specified in the problem input and writes the information on a magnetic tape to be used by the main RBU program. In addition to the basic library and problem input, a tape, containing a cumulation of all previous output of the Cross Section Preparation Program which pertained to the same energy group structure as the present problem, is used by the code. The program then makes use of any of the necessary information that happens to be already available on the cumulative tape and, in addition to the tape required for a particular problem, produces a new cumulative tape. The essential data, aside from the basic library to be supplied to the cross section preparation routine is: the energy limits of the microscopic groups, list of isotopes initially present in the reactor, and the ambient temperatures in the regions in which these isotopes are. Using this information and the basic library, the routine determines any additional isotopes which will appear in the reactor during operation as a result of burnup and it computes the average cross sections for each microscopic energy group for each of the isotopes to be required. The temperature is used in the calculation of Doppler broadened resonances.

In addition to this essential information, some additional data may be supplied for the treatment, in the monte carlo part of the calculation, of low energy scattering. For those isotopes requiring it, special atomic weights for use in the center of mass-laboratory system conversion on near thermal collisions may be given and probability distributions of velocity increments to be added to the emergent velocities in such collisions may be supplied. The special atomic weights consist of a set of G_q numbers to be used in groups I- G_q through I for the q^{th} isotope in the input. The probability distributions are given in the form of a table of probabilities and velocity increments for each of several distributions; the distribution to be used for a particular isotope is identified by specifying with the isotope's input data an index

referring to the appropriate table. An index of zero associated with an isotope signifies that velocity increments need not be used for it.

The basic library consists of a section of general nuclear data and specific sections giving the necessary cross section information about each isotope. The general nuclear data includes a table giving all the descendants, direct and indirect of each isotope in the library, and a table of the direct descendants only of each isotope with an index indicating whether the transformation is the result of neutron capture, $(n, 2n)$, fission, or radioactive decay reactions. The index indicating fission may have one of six values to indicate which of the six fission yields given with the parent isotope data applies to this particular descendant. In addition, the general nuclear data includes ten tables of spectra for inelastic collisions. An index may be given for each isotope in the isotope data selecting one of these tables to be associated with it. Also included in the general nuclear data are twenty sets of resonance structure parameters. Each set includes values of Γ_n , Γ_f , Γ_γ , g and E_0 for each of twenty resonances, a value of v_{fr} and σ_p for all resonances for isotopes to which the set applies and a value of $\bar{\Gamma}_n$, $\bar{\Gamma}_\gamma$, $\bar{\Gamma}_f$, g and D for the unresolved resonances. An index associated with each isotope indicates which set is to be used for it.

The data associated with a particular isotope in the basic library consists of a general section and a section giving the energy dependent properties. The general data includes the isotope's name or index, its atomic weight, six fission yields, the mean lifetime for radioactive decay, the energy below which elastic scattering is isotropic, the potential scattering cross section for use in resonances, either an index selecting one of the inelastic spectrum tables or a level spacing for use in the evaporation model inelastic spectrum, and an index selecting one of the sets of resonance parameters.

The energy dependent data is given for a set of ranges the widths of which vary from range to range and from isotope to isotope, being chosen as is appropriate to the range and isotope in question.

With each range (for each isotope) is associated an index, δ , identifying the manner in which the properties vary within that range. The possible types of variation are described in Table I.

TABLE I

VARIATION OF CROSS SECTIONS WITHIN THE ENERGY RANGE $E_n \leq E \leq E_{n-1}$

Quantity	$\delta = 1$	$\delta = 2$	$\delta = 3$	$\delta = 4$	$\delta = 5$	$\delta = 6$
σ_{el}	Linear	Constant	Constant	Breit Wigner	<div style="display: inline-block; vertical-align: middle;"> <div style="display: inline-block; vertical-align: middle;">Breit Wigner</div> <div style="display: inline-block; vertical-align: middle;">With random</div> <div style="display: inline-block; vertical-align: middle;">Widths</div> </div>	<div style="display: inline-block; vertical-align: middle;"> <div style="display: inline-block; vertical-align: middle;">Same as 4</div> <div style="display: inline-block; vertical-align: middle;">but reso-</div> <div style="display: inline-block; vertical-align: middle;">nance para-</div> <div style="display: inline-block; vertical-align: middle;">meters</div> <div style="display: inline-block; vertical-align: middle;">rather than</div> <div style="display: inline-block; vertical-align: middle;">group aver-</div> <div style="display: inline-block; vertical-align: middle;">ages are</div> <div style="display: inline-block; vertical-align: middle;">stored for</div> <div style="display: inline-block; vertical-align: middle;">direct cal-</div> <div style="display: inline-block; vertical-align: middle;">culation in</div> <div style="display: inline-block; vertical-align: middle;">monte carlo</div> <div style="display: inline-block; vertical-align: middle;">program</div> </div>
σ_c	Linear	Linear	$\frac{1}{V}$	Breit Wigner		
σ_f	Linear	Linear	$\frac{1}{V}$	Breit Wigner		
σ_{inel}	Linear	Linear	Assumed not present	Assumed not present	Assumed not present	
ν_f	Constant	Constant	Constant	Constant	Constant	
ν_{inel}	Constant	Constant	Assumed not present	Assumed not present	Assumed not present	
a_0	Constant	Constant	Constant	Constant	Assumed not present	Assumed not present
a_1	Constant	Constant	Constant	Constant	Assumed not present	Assumed not present
a_2	Constant	Constant	Constant	Constant	Assumed not present	Assumed not present

In Table I the term linear means that the cross section is assumed to have the form

$$\sigma(E) = \sigma_n + \frac{\sigma_{n-1} \cdot \sigma_n}{E_{n-1} - E_n} (E - E_n)$$

$$E_n \leq E \leq E_{n-1} \quad (127)$$

The term $\frac{1}{V}$ means that

$$\sigma(E) = \frac{\sigma_n}{E^{1/2}}$$

$$E_n \leq E \leq E_{n-1} \quad (128)$$

The term Breit Wigner if $\delta = 4$ means that

$$\begin{aligned}\sigma_s(E) &= \sigma_{s_o} \psi(X, \theta) + 2 \left(\frac{a+1}{a} \right) \sqrt{\sigma_p \sigma_{s_o}} g(X, \theta) + \sigma_p \\ \sigma_c(E) &= \frac{\sigma_{c_o}}{\sqrt{E}} \psi(X, \theta) \\ \sigma_f(E) &= \frac{\sigma_f}{\sqrt{E}} \psi(X, \theta)\end{aligned}\quad (129)$$

where

$$\begin{aligned}X &= \frac{2 \left[\left(\frac{a}{a+1} \right) E - E_o \right]}{\Gamma} \\ \theta &= 3.446 \times 10^{-4} \frac{ET}{A\Gamma^2} \left(\frac{a}{a+1} \right)^2 \\ \psi(X, \theta) &= \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{e^{-(X-Y)^2/4\theta}}{1+Y^2} dy \\ \chi(X, \theta) &= \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} \frac{y e^{-(X-Y)^2/4\theta}}{1+Y^2} dy \\ \sigma_{s_o} &= \frac{2.607 \times 10^6}{(\Gamma_n + \Gamma_\gamma + \Gamma_f)^2} \frac{\Gamma_n^2}{E_o} g\left(\frac{1+a}{a}\right) \\ \sigma_{c_o} &= \frac{2.607 \times 10^6}{(\Gamma_n + \Gamma_\gamma + \Gamma_f)^2} \frac{\Gamma_n}{\sqrt{E_o}} \Gamma_\gamma g\left(\frac{1+a}{a}\right)^{3/2} \\ \sigma_{f_o} &= \frac{\Gamma_f}{\Gamma_\gamma}\end{aligned}\quad (130)$$

Equations (129) and (130) are derived in Appendix D. The evaluation of ψ and χ is described in Appendix C. In the integration of Breit Wigner Cross Sections over a range $E_n \leq E \leq E_{n+1}$, for $\delta = 4$ the functions are evaluated at ten points within the range and integrated by Simpson's Rule.

When $\delta = 6$ the cross sections are evaluated in the monte carlo portion of the main program using Equation (22) which is equivalent to (130) except for the addition of factors to account for the higher angular momentum states. These factors are negligibly different from unity for the energy ranges in which the resonances are resolved.

APPENDIX A
QUANTITIES REQUIRED AND PRODUCED
IN THE MAIN PORTIONS OF THE PROGRAM

1. CROSS SECTION PREPARATION ROUTINE INPUT

A. BASIC LIBRARY

1. General Nuclear Data

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>
Table of descendants	Table containing list of all isotopes in library, each followed by a list of all its direct and indirect descendants.	1 table
Table of direct descendants	Table containing list of all isotopes in library, each followed by a list of all its direct descendants with the mode of production given with each descendant.	1 table
$(P_{in}, V_{in}^2)_D$	Table of probabilities that an in-elastically scattered neutron be emitted with square of velocity in center of mass system diminished by corresponding V_{in}^2 . Each table contains 16 P_{in} and V_{in}^2 .	10 tables
D_{R0}	Average energy spacing between unresolved resonances for ρ^{th} table of resonance parameters	One for each of twenty tables
$\bar{\Gamma}_{n00}$	Average reduced neutron partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of twenty tables
$\Gamma_{\gamma0}$	Radiation partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of twenty tables
$\bar{\Gamma}_{f0}$	Average fission partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of twenty tables

g_{ρ}	Statistical weight for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of twenty tables
$\nu_{f\rho}$	Number of neutrons emitted per fission for resonances for ρ^{th} table of resonance parameters.	One for each of twenty tables
$\sigma_{p\rho}$	Potential scattering cross section for resonances for ρ^{th} table of resonance parameters	One for each of twenty tables
$E_{0\rho\tau}$	Energy value at the maximum of the τ^{th} resolved resonance of the ρ^{th} table of resonance parameters.	One for each of twenty resolved resonances for each of twenty tables
$\Gamma_{n\rho\tau}$	Neutron partial width at $E_{0\rho\tau}$ for the τ^{th} resolved resonance of the ρ^{th} table of resonance parameters.	One for each of twenty resolved resonances for each of twenty tables
$\Gamma_{\gamma\rho\tau}$	Radiation partial width for the τ^{th} resolved resonance of the ρ^{th} table of resonance parameters.	One for each of twenty resolved resonances for each of twenty tables
$\Gamma_{f\rho\tau}$	Fission partial width for the τ^{th} resolved resonance of the ρ^{th} table of resonance parameters.	One for each of twenty resolved resonances for each of twenty tables
$g_{\rho\tau}$	Statistical weight for the τ^{th} resolved resonance of the ρ^{th} table of resonance parameters.	One for each of twenty resolved resonances for each of twenty tables

2. Isotope Data

a	Isotope name.	1 for each isotope
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(any inel)_a
 (any abs)_a
 (any r.r.)_a
 (any f)_a

Statements indicating whether there are for isotope a any inelastic or any absorption cross sections, any resonance range, any fission cross section.

1 each for each isotope

α_a

Atomic weight of isotope a.

1 for each isotope

ρ_a

Table of resonance parameters to use with isotope a.

1 for each isotope

γ_{ta}

Fraction of fission cross section which is cross section for production of the tth fission product isotope.

6 for each isotope

λ_a

Mean lifetime for radioactive decay.

1 for each isotope

E_{aniso_a}

Energy below which elastic scattering is isotropic in the center of mass system.

1 for each isotope

D_a

Either the resonance spacing used in computing spectrum of inelastically scattered neutrons for isotopes which use the evaporation model, or a value of an index identifying the inelastic spectrum table to be used, is given.

1 for each isotope

P_a

Identification number of list of resolved resonance parameters to be used with isotope a.

1 for each isotope

3. Energy Range Data

E_{na}

Energy values at which cross sections are specified for isotope a.

N for each isotope

δ_{na}

Index indicating type of cross section (or similar quantity) variation in nth range of isotope a.

N for each isotope

$\sigma_{el\ an}$	Elastic scattering cross section.	} 1 for each isotope and energy range with $\delta=1, 2$, or 3
$\sigma_{c\ an}$	Capture cross section.*	
$\sigma_{f\ an}$	Fission cross section.*	
$\nu_{f\ an}$	Number of neutrons emitted per fission.*	
$\sigma_{inel\ an}$	Inelastic scattering cross section.*	
$\nu_{inel\ an}$	Number of neutrons emitted per inelastic scattering.*	1 for each isotope and energy range with $\delta = 1, 2$, or 3
$a_{0\ an}, a_{1\ an}, a_{2\ an}, a_{3\ an}$	Coefficients of powers of μ for differential elastic scattering cross section.	1 for each isotope and energy range, E_n above E_{aniso}
$\left. \begin{array}{l} \Gamma_{n\ an}, \Gamma_{\gamma\ an}, \Gamma_{f\ an}, \\ \nu_f, E_{0\ an}, g_{an} \end{array} \right\}$	Special quantities used instead of cross sections when $\delta = 4$. E_0 is the energy at the maximum of the resonance Γ_n , Γ_{γ} , and Γ_f are the neutron, radiative capture and fission widths respectively. The statistical weight is g . The number of neutrons emitted per fission is ν_f . **	1 for each isotope and energy range with $\delta = 4$

B. PROBLEM INPUT

1. General Problem Data

Q	Number of isotopes listed in input for which group cross sections are to be made.	1
I	Number of monte carlo groups.	1

* These appear only if corresponding (any-) _a is yes.

** Each of these appear regardless of the corresponding (any-) _a.

E_i	Lower energy limit of group i.	I
$\overline{H}$	Number of tables of velocity increment probability distributions for near thermal scattering.	1
$(P_{th}, \Delta V_{th})_{\xi}$	Table of probabilities that the incremental velocity added vectorially to a neutron's velocity after a near thermal collision as a result of the thermal motion of the target will be less than or equal to the corresponding ΔV_{th} . Each table contains 16 P_{th} and ΔV_{th} ($\Delta V_{th_0} = 0$ for all tables).	$\overline{H}$

2. Isotope Data

a_q	Name of a required isotope.	1 for each isotope to be used (Q isotopes)
T_q	Temperature for the material containing the q^{th} isotope.	Q
G_q	Number of monte carlo groups for which special low energy atomic weights are given.	Q
a_{iq}	Special atomic weights for lowest G monte carlo groups for q^{th} isotope.	G_q for q^{th} isotope
ξ_q	Identification number of table of thermal velocity increment probability distribution to be used with isotope q.	Q

II. MONTE CARLO INPUT

A. MONTE CARLO SYSTEM DATA

(In the following table it is to be understood that similar data is required for each monte carlo system.)

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>
s	System identification number.	1
T ₀	Time at which equilibrium is assumed to be established so that tallying of results begins.	1
T	Census time.	1
I	Number of microscopic groups.	1
H	Number of microscopic regions.	1
H'	Number of outer regions used in defining the limits of system s.	1
F	Number of region sets.	1
J	Number of macroscopic groups.	1
J'	Number of macroscopic groups included in random resonance range.	1
K	Number of macroscopic regions in system s.	1
M	Number of materials.	1
S'	Number of inelastic spectrum tables	1
E	Number of thermal velocity increment tables.	1
R	Total number of distinct elastic scattering cross sections.	1
B	Total number of boundaries.	1
W	Total number of resonance scatterers.	1
N _{MC}	Number of particles to be followed.	1
N' _{MC}	Number of diffusion time steps between monte carlo calculations.	1

R'	Number of distinct inelastic scattering cross sections.	1
I_{aniso}	Total number of sets of anisotropic scattering coefficients.	1
P	Number of tables of resonance parameters.	1
$(P_{\text{in}}, V_{\text{in}}^2)_D$	Table of probabilities that an inelastically scattered neutron be emitted with square of velocity in center of mass system diminished by corresponding V_{in}^2 . Each table contains 16 P_{in} and V_{in}^2 .	S'
$(P_{\text{th}}, \Delta V_{\text{th}})_\xi$	Table of probabilities that the incremental velocity added vectorially to a neutron's velocity after a near thermal collision as a result of the thermal motion of the target will be less than or equal to the corresponding ΔV . Each table contains 16 P_{th} and ΔV_{th} ($\Delta V_{\text{th}0} = 0$ for all tables).	H
$D_{R\rho}$	Average energy spacing between unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$\bar{\Gamma}_{n0\rho}$	Average reduced neutron partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$\Gamma_{\gamma\rho}$	Radiation partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$\bar{\Gamma}_{f\rho}$	Average fission partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables
g_ρ	Statistical weight for unresolved resonance for ρ^{th} table of resonance parameters.	One for each of P tables
$\nu_{f\rho}$	Number of neutrons emitted per fission for resonances for ρ^{th} table of resonance parameters.	One for each of P tables
σ_p	Potential scattering cross section for resonances for ρ^{th} table of resonance parameters.	One for each of P tables

$E_{0\rho\tau}$	Energy value at the maximum of the τ^{th} resolved resonance for the ρ^{th} table of resonance parameters.	One for each of twenty resolved resonances for each of P tables
$\Gamma_{n\rho\tau}$	Neutron partial width for the ρ^{th} table of resonance parameters and the τ^{th} resonance.	One for each of twenty resolved resonances for each of P tables
$\Gamma_{\gamma\rho\tau}$	Radiation partial width for the ρ^{th} table of resonance parameters and the τ^{th} resonance.	One for each of twenty resolved resonances for each of P tables
$\Gamma_{f\rho\tau}$	Fission partial width for the ρ^{th} table of resonance parameters and the τ^{th} resonance.	One for each of twenty resolved resonances for each of P tables
$g_{\rho\tau}$	Statistical weight for the ρ^{th} table of resonance parameters and the τ^{th} resonance.	One for each of twenty resolved resonances for each of P tables

B. BOUNDARY DATA

b	Boundary identification number.	B
D_b	Boundary type for boundary b.	B
$A_b, B_b, C_b,$ $x_{o_b}, y_{o_b}, z_{o_b}, K_b$	Parameters in the boundary equation $A(x-x_o)^2+B(y-y_o)^2+C(z-z_o)^2-K=0$	1 each per boundary
ω_b	Albedo of boundary b.	B

C. MICROSCOPIC REGION DATA

h	Region identification number.	H
k_h	Macroscopic region in which h is contained.	H
f_h	Region set which includes region h.	H

B_h	Number of boundaries defining region h.	H
b_h	A boundary of region h.	B_h for each region
g_{b_h}	Sense of boundary b_h with respect to region h.	B_h for each region
$\perp_{b_h}$	Indicator telling whether or not crossings of boundary b_h from region h contribute to perpendicular leakage cross section in macroscopic region containing h for diffusion calculation.	B_h for each region
q_{b_h}, q'_{b_h}	Regions in order of likelihood into which a neutron is expected to go if it crosses boundary b_h from region h. ($q'_{b_h} = 0$ indicates such neutrons can only go into q_{b_h} .)	B_h each for each region
m_h	Material contained in region h.	H
I_h	Importance of region h.	H

D. MATERIAL DATA

m	Material identification number.	M
T_m	Temperature of material m.	M
f_m	Indicator telling whether or not there is a fission cross section in material m.	M
$P_{f_{mi}}$	Number of neutrons per collision in group i, material m emitted as a result of fission.	I for each material for which f_m is yes
R_m	Number of distinct elastic scattering cross sections in material m.	M
$P_{el_{r_{mi}}}$	Number of neutrons per collision in group i, material m emitted as a result of elastic scattering associated with r^{th} elastic scattering cross section.	$I \times R_m$ for each material

a_{rm_i}	Atomic weight associated with the r^{th} elastic cross section in group i , material m .	$I \times R_m$ for each material
R'_m	Number of distinct inelastic scattering cross sections in material m .	M
$P_{inel_{r'mi}}$	Number of neutrons per collision in group i , material m emitted as a result of inelastic scattering associated with r^{th} inelastic scattering cross section.	$I \times R'_m$ for each material
$D_{r'm}$	Inelastic spectrum table identification number or resonance spacing for inelastic spectrum nuclear temperature calculation associated with r'^{th} inelastic scattering cross section in region m .	R'_m for each material
λ_{mi}	Mean free path in material m , group i .	$I \times M$
ξ_{rm}	Identification number of table of velocity increments for near thermal scattering associated with r^{th} elastic cross section in material m .	R_m for each material
$I_{aniso_{rm}}$	Group number of lowest energy group in which scattering associated with the r^{th} elastic scattering cross section is anisotropic.	R_m for each material
W_m	Number of resonance scatterers in material m .	M
$I_{1_{wm}}, I_{2_{wm}}$	Minimum and maximum velocity group numbers for random resonances for the w^{th} resonance scatterer in material m .	W_m each for each material
$I_{3_{wm}}$	Maximum velocity group numbers for resolved resonances for the w^{th} resonance scatterer in material m . $I_{2_{wm}}$ is the corresponding minimum group number.	W_m each for each material

ϵ_{wm}	Identification of the table of resonance parameters to be used with the w^{th} resonance scatterer in material m .	W_m for each material
N_{wm}	Atomic concentration of the w^{th} resonance scatterer in material m .	W_m for each material
$a_{0_{rmi}}, a_{1_{rmi}}, a_{2_{rmi}}, a_{3_{rmi}}, a_{M_{rmi}}$	Coefficients of powers of μ of differential scattering cross section for r^{th} elastic scatterer in group i , material m . The maximum value of this power series is a_M .	$I_{aniso_{rm}}$ for each r in each material

D. GROUP DATA

i	Identification number of group.	I
V_i	Maximum velocity of group i .	I
I_i	Importance of group i .	I
j_i	Macroscopic group in which group i is contained.	I

E. TIME STEP DATA

t	Identification number of monte carlo time step.	--
A_{ih}^t	Sampling factor for initial particles entering the t monte carlo time step in group i , region h .	$I \times H$ for each monte carlo time step

III. DIFFUSION CALCULATION INPUT

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>	<u>Calculated in</u>
D_{jk}	Diffusion coefficient.	KJ	Prediff
T_{jk}	Removal cross section.	KJ	Prediff
$T_{jj',k}$	Transfer cross section.	K/2 J(J-1)	Prediff
$F_{j,k}$	Fission neutron production cross section.	KJ	Prediff
χ_j	Fission spectrum coefficient.	J	Initial org.
$\phi_{n,j}^{t-\Delta t}$	Fluxes from previous time step.	NJ	Diff.
$\lambda^{t-\Delta t}$	Multiplication constant from previous time step.	1	Diff.
$P_n^{t-\Delta t}$	Fission source densities from previous time step.	N+K	Diff.
Δr_k	Mesh space in region k.	K	Input
N_k	Number of mesh spaces in region k.	K	Input
B_{o_j}	Boundary conditions at origin.	J	Input
R_o	Coordinate of first mesh point.	1	Input
B_{N_j}	Boundary conditions at outer coordinate.	J	Input
ω	Acceleration factor.	1	Input
ϵ_3	Convergence test tolerance for λ .	1	Input
ϵ_4	Convergence test tolerance for P_n .	1	Input
ρ	Geometry Index.	1	Input

J	Number of macroscopic groups.	1	Input
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K	Number of macroscopic regions.	1	Input
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IV. BURNUP INPUT

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>	<u>Calculated in</u>
t	Time.	1	BU
Δt	Basic time step.	1	BU
M	Total number of materials in problem.	1	Input
ϵ_1	Tolerance limit for increase of time step.	1	Input
ϵ_2	Tolerance limit for decrease of time step.	1	Input
N_{BU_m}	Number of diffusion calcu- lations between burnup steps on material m .	M	BU (& Input)
π_m	Number of diffusion calcu- lations since last concen- tration calculation on material m .	M	BU
ρ_m	Number of backward differ- ences of rates of change of concentration available for concentration predictions for each isotope in material m .	M	BU
t_{ρ_m}	Time for which the last con- centration predictions in region m were made.	M	BU
N_q^{p-1}	Concentration of q^{th} iso- tope of material m at $t_{\rho_m} - N_{BU_m} \Delta t$	Q_m for each m	BU
$\nabla_{N_{qm}}^i$ $i=0,1,2,3$	Backward differences of rate of change of concen- tration of q^{th} isotope of material m at $t_{\rho_m} - N_{BU_m} \Delta t$.	Up to $3Q_m$ for each m	BU

M_{ρ}	Number of materials on which burnup calculation will be made at t.	1	Pre BU
N_{qm}^{ρ}	Concentration of q^{th} isotope of material m predicted for time t.	Q_m for each m of M_{ρ}	BU
Q_m	Number of isotopes in material m.	M_{ρ}	Cross section Ave Rtn
$D_{q,m}$	The number of daughters of the q^{th} isotope of material m.	Q_m for each of M_{ρ} 's	Cross Section Ave Rtn
$F_{q'qm}$	Production rate of the q^{th} isotope in material m per unit concentration of the q'^{th} ($q' \neq q$).	$D_{q'm}$ for each isotope of M_{ρ} 's	Pre BU
E_{qm}	Consumption rate of the q^{th} isotope in material m per unit concentration (of itself).	Q_m for each of M_{ρ} 's	Pre BU

V. CROSS SECTION PREPARATION PROGRAM OUTPUT

A. GENERAL DATA

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>
Q	Number of isotopes or cross section sets present in output.	1
I	Number of monte carlo groups.	1
—	Table of direct descendants and modes of formation.	1
E_1, V_{i+1}	Lower energy and velocity limit of group i.	1 each
Ξ	Number of tables of velocity increment probability distributions for near thermal scattering present in output.	1
$(P_{th}, \Delta V_{th})_{\xi}$	Table of velocity increment probability distributions. Each table contains 16 P_{th} and 17 ΔV_{th} ($\Delta V_{th_0} = 0$ for all tables).	Ξ tables
S'	Number of tables of inelastic spectra present in output.	1
$(P_{in}, V_{in}^2)_s$	Table of inelastic spectrum. Each table contains 16 P_{in} and 17 V_{in} .	10 tables
P	Number of tables of resonance parameters.	1
$D_{R\rho}$	Average energy spacing between unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$\bar{\Gamma}_{n0\rho}$	Average reduced neutron partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables

$\Gamma_{\gamma\rho}$	Radiation partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$\bar{\Gamma}_{f\rho}$	Average fission partial width for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of
g_{ρ}	Statistical weight for unresolved resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$\nu_{f\rho}$	Number of neutrons emitted per fission for resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$\sigma_{p\rho}$	Potential scattering cross section for resonances for ρ^{th} table of resonance parameters.	One for each of P tables
$E_{0\rho\tau}$	Energy value at the maximum of the τ^{th} resolved resonance for the ρ^{th} table of resonance parameters.	One for each of twenty resolved resonances for each of P tables
$\Gamma_{n\rho\tau}$	Neutron partial width for the ρ^{th} table of resonance parameters and the τ^{th} resolved resonance	One for each of twenty resolved resonances for each of P tables
$\Gamma_{\gamma\rho\tau}$	Radiation partial width for the ρ^{th} table of resonance parameters and the τ^{th} resolved resonance.	One for each of twenty resolved resonances for each of P tables
$\Gamma_{f\rho\tau}$	Fission partial width for the ρ^{th} table of resonance parameters and the τ^{th} resolved resonance.	One for each of twenty resolved resonances for each of P tables
$g_{\rho\tau}$	Statistical weight for the ρ^{th} table of resonance parameters and the τ^{th} resolved resonance.	One for each of twenty resolved resonances for each of P tables

B. ISOTOPE DATA

a_q	Isotope name.	Q
T_q	Temperature for the material containing isotope a_q .	Q
G_q	Number of groups for which special low energy atomic weights are given for a_q .	Q
a_{iq}	Special atomic weights for lowest G_q monte carlo groups for a_q .	G_q for each isotope
t_q	Identification number of table of thermal velocity increment probability distribution to be used with a_q .	Q
ρ_q	Identification number of table of resonance parameters to be used with isotope q .	Q
$\left. \begin{array}{l} \text{(any inel)}_q \\ \text{(any abs)}_q \\ \text{(any r.r.)}_q \\ \text{(any f)}_q \end{array} \right\}$	Statements indicating whether there are for a_q any inelastic or absorption cross sections, any resonance range, any fission cross section.	Q each
a_q	Atomic weight of a_q .	Q
y_{tq}	Fraction of fission cross section a_q which is cross section for production of t^{th} fission product isotope.	6Q
λ_q	Mean lifetime for radioactive decay of a_q .	Q
$I_{\text{aniso } q}$	Group number of lowest group for which there is anisotropic scattering by a_q .	Q
D_q or $S_q = 0, 1, \dots$	Resonance spacing for inelastic spectrum or identification number of inelastic spectrum table.	$\sum_m R'_m$
I_1, I_2, I_3	Upper and lower group number limits for unresolved resonances in a_q (I_2 and I_1) and upper and lower group number limits for resolved resonances in a_q (I_3 and I_2).	1 each for each isotope for which (any r.r.) is yes

C. GROUP DATA

$\sigma_{el\ qi}$	Elastic scattering cross section of a_q in group i.	1xQ
$\sigma_{c\ qi}$	Capture cross section of a_q in group i. Given only if (any abs) is yes.	I for each isotope for which (any abs) is yes
$\sigma_{f\ qi}$	Fission cross section of a_q in group i. Given only if (any f) is yes.	I for each isotope for which (any f) is yes
$(\nu_f \sigma_f)_{qi}$	Product of number of neutrons emitted per fission and microscopic fission cross section in group i for a_q .	I for each isotope for which (any f) is yes.
$\sigma_{n,2n\ qi}$	n, 2n cross section of a_q in group i.	20 for each isotope for which (any inel) is yes
$(\nu_{inel} \sigma_{inel})_{qi}$	Product of number of neutrons emitted per inelastic scattering and microscopic fission cross section in group i for a_q .	20 for each isotope for which (any inel) is yes
$\sigma_{T\ qi}$	Microscopic total cross section in group i for a_q .	1xQ
$a_{0\ qi}, a_{1\ qi}, a_{2\ qi}, a_{3\ qi}$	Coefficients of powers of μ for anisotropic scattering in group i for A_q .	I _{aniso_q} each for each isotope

D. PRINT OUT

$\left. \begin{array}{l} a_q \\ T_q \\ G_q \\ \xi_q \end{array} \right\}$	Isotope name, temperature, number of special atomic weights, and identification number of thermal increment table associated with q^{th} isotope.	Q each
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VI. MONTE CARLO OUTPUT*

A. SYSTEM DATA**

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>
N_{IV}	Number of initial neutrons.	1
N_{CV}	Number of census neutrons.	1
n_{IV}	Number of initial particles.	1
n_{CV}	Number of census particles.	1
N_C	Number of neutrons going into collisions.	1
N_e	Number of neutrons emerging from collisions.	1
N_B	Number of neutrons going into boundaries minus number emerging (non-outer boundaries).	1
N_{BO}	Number of neutrons going into boundaries minus number reflected (outer boundaries).	1
N'_e	Sum of P'_s for all neutrons entering collisions.	1
$\langle N_{BO} \rangle$	Expectation values of leakage multiplied by $(1-\omega)$.	1
$\langle N_c \rangle$	Expectation value of neutrons going into collisions.	1
$\langle N'_e \rangle$	Expectation value of number of neutrons emerging from collisions.	1

* In all that follows under subject VI, the subscript s is implied and a per monte carlo system is implied in the Number Required column.

** With the exception of n_{CV} , the data included under subject VI-A is used purely for program and input checking. This information is printed out after each monte carlo time step.

B. MACROSCOPIC DATA

$\begin{aligned} &(\Sigma_s \phi)_{wmj} / \phi_{wm} \\ &(\Sigma_c \phi)_{wmj} / \phi_{mj} \\ &(\Sigma_f \phi)_{wmj} / \phi_{mj} \end{aligned}$	<p>Number of scattering, capture, and fission collisions in the resonance range of diffusion group j for w^{th} random resonance scatterer in material m per unit neutron flux in material m and group j.</p>	<p>(Number of j groups covering random resonance range) $\times W_m$ each for each material</p>
L_{kj}	<p>Surface integral of current from macroscopic group j and region k on boundaries separating k from another macroscopic region of the reactor.</p>	<p>KxJ</p>
$(\hat{n} \cdot \vec{\nabla} \phi)_{kj}$	<p>Surface integral of normal gradient of the flux in group j over boundaries separating k from other macroscopic regions of the reactor.</p>	<p>KxJ</p>
$\mathcal{L}_{kj} / \phi_{kj}$	<p>Leakage from the reactor perpendicular to the direction of investigation of the diffusion calculation from group j, region k per unit neutron flux in macroscopic region k and group j.</p>	<p>KxJ</p>

C. MICROSCOPIC DATA

ϕ_{if}	<p>Total neutron flux in group i, region set f normalized to one neutron centimeter per time step in the macroscopic region containing f.</p>	<p>IxH</p>
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VII. DIFFUSION CALCULATION OUTPUT

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>
p_n^t	Fission source density at time t and mesh point n.	N+K
ϕ_{nj}^t	Neutron flux density in group j at mesh point n, and time t per unit energy and per unit volume where the volume element in $r^U dr$.	NJ
k_t	Multiplication constant at time t.	1

VIII. BURNUP OUTPUT

<u>Symbol</u>	<u>Definition</u>	<u>Number Required</u>
t	Time.	1
Δt	Basic time step.	1
N_{BU_m}	Number of diffusion calculations between burnup steps on material m.	M
π_m	Number of diffusion calculations since last concentration prediction on material m.	M
ρ_m	Number of backward differences of rates of change of concentration available for concentration predictions for isotopes in material m.	M
t_{ρ_m}	Time for which last concentration predictions in material m were made.	M
$N_{qm}^{\rho-1}$	Concentration of q^{th} isotope of material m at $t_{qm} - N_{BU_m} \Delta t$.	Q_m for each m
$\nabla^i N_{qm}$ $i=0,1,2,3$	Backward differences of rates of change of concentration of q^{th} isotope of material m at $t_{\rho_m} - N_{BU_m} \Delta t$.	Up to $3Q_m$ for each m
N_{qm}^{ρ}	Concentration of q^{th} isotope of material m predicted for time t_{ρ_m}	Q_m for each of M_{ρ} m's

APPENDIX B
SELECTION FROM PROBABILITY DISTRIBUTIONS

1. RANDOM NUMBERS

The process basic to all random selection techniques in RBU is the choosing of a number from a universe of numbers uniformly distributed between zero and one. Because of the importance of numbers selected from this distribution, they are generally called simply random numbers in discussions of monte carlo calculations. As in virtually all monte carlo calculations the method is not actually random but involves the use of a recipe which leads to numbers which collectively have the properties of a set chosen by a random process; these are generally called pseudo-random numbers. The properties of importance here are that the mean of any reasonably large sample approaches the mid point of the sample range as the sample size increases, that they are distributed over the range with adequate fineness that the frequencies of lengths of increasing and decreasing chains be distributed in the same way as those of actually random numbers and that no obvious regularities occur. It is usual to require also that the cycle length of the process be relatively long and it is, of course, also important that the process involve only a very small amount of computing time. In general, because of the complexity of monte carlo calculations, it is desirable to apply more rigid requirements than appear superficially to be necessary in selecting a random number generator.

A method which has been shown theoretically to produce numbers having the properties of those obtained from a random selection is the multiplicative method. In this technique

$$R_{n+1} = (k R_n) \bmod \rho \quad (B-1)$$

where k and R_0 have certain properties and ρ is the word length of the computer. In RBU

$$\begin{aligned} k &= 5^{15} \\ R_0 &= (247162405723)_8 \\ \rho &= 2^{35} \end{aligned} \quad (B-2)$$

II. SELECTION OF DISTANCE TO COLLISION

The selection of the number of mean free paths a particle will travel before a collision is made from the distribution

$$\frac{dP(S/\lambda)}{d(S/\lambda)} = -e^{-S/\lambda} \quad (B-3)$$

The method is based on the fact that equal increments in the logarithm of the cumulative probability represent equal intervals in the argument.. It consists of selecting an interval in the logarithm of P by repetitive comparison of a random number with 0.5. For each successive random number less than 0.5, the natural logarithm of two is added to the upper and lower limits of the range from which S/λ is to be selected. The sequence of comparisons is stopped on the first random number greater than 0.5 thus determining an interval within which S/λ is to be selected. A final random number determines, by a table lookup which of eight possible values within the interval is used.

III. RANDOM COSINES

The direction cosines are determined by a method which avoids the necessity of evaluating trigonometric functions just as the previous technique avoided logarithms. To do this α , β , and γ are defined in terms of spherical coordinates

$$\begin{aligned}\alpha &= \cos \phi \sin \theta \\ \beta &= \sin \phi \sin \theta \\ \gamma &= \cos \theta\end{aligned}\tag{B-4}$$

The value of γ is then selected as a random number between -1 and +1 by

$$\gamma = 2\xi_1 - 1\tag{B-5}$$

where ξ_1 is uniformly distributed between 0 and 1. Two more random numbers ξ_2 and ξ_3 are selected. These are accepted only if the sum of their squares is less than or equal to unity; otherwise two more are chosen until this condition is fulfilled. The ratio

$$\frac{\xi_2}{\xi_3}$$

is then the tangent of an angle ϕ , randomly chosen from a universe uniformly distributed between 0 and $\frac{\pi}{2}$. Finally,

$$\begin{aligned}\alpha &= \pm \xi_3 \sqrt{\frac{1-\gamma^2}{\xi_2^2 + \xi_3^2}} \\ \beta &= \pm \xi_2 \sqrt{\frac{1-\gamma^2}{\xi_2^2 + \xi_3^2}}\end{aligned}\tag{B-6}$$

where the two signs are determined by selection of two random bits.

Although this method appears complicated, it is, due to its efficiency, faster than the obvious method of choosing and normalizing three random numbers the sum of whose squares is less than or equal to unity.

IV. SELECTION OF RESONANCE PARTIAL WIDTHS

The fission width is distributed as

$$dP(v) = e^{-v} dv \quad (B-7)$$

where

$$v = \frac{\Gamma_f}{\Gamma_f}$$

Selection of v then is by the same method as that of the number of mean free paths to collision described above.

The reduced neutron width is distributed as

$$dP(u) = \sqrt{\frac{2}{\pi}} e^{-u^2/2} du \quad (B-8)$$

where

$$u = \left(\frac{\Gamma_{no}}{\Gamma_f} \right)^{1/2}$$

The method used in RBU is to select two random numbers L_1 and L_2 from an exponential distribution as in the selection of a distance to collision above. If $(L_1 - 1)^2 \leq 2 L_2$, u is taken to be equal to L_1 . Otherwise two more random logarithms are selected and the process repeated until a pair satisfying the condition is found.

The probability that an L_1 will be obtained and accepted is

$$\begin{aligned} P_{acc}(L_1) &= \int_{(L_1-1)^2/2}^{\infty} P(L_1) P(L_2) dL_2 \\ &= e^{-L_1} \int_{(L_1-1)^2/2}^{\infty} e^{-L_2} dL_2 \end{aligned} \quad (B-9)$$

which corresponds to (B-8).

V. SELECTION FROM THE EVAPORATION MODEL INELASTIC SPECTRUM

The probability distribution is

$$dP(E) = CE e^{-E/T} dE \quad (B-10)$$

The sum of two random logarithms has the distribution

$$P(X) = \int_0^X e^{-Y} e^{-(X-Y)} dY = X e^{-X} \quad (B-11)$$

Thus the sum of two numbers, X and Y , each distributed as $E^{-E/T}$ has the distribution required.

APPENDIX C THE CALCULATION OF PSI AND CHI

I GENERAL

Psi and Chi are defined as follows:

$$\psi(x, 0) = \frac{1}{\sqrt{4\pi\theta}} \int_{-\infty}^{\infty} \frac{\exp[-(Y-X)^2/4\theta]}{1+Y^2} dY \quad (C-1)$$

$$\chi(x, 0) = \frac{1}{\sqrt{4\pi\theta}} \int_{-\infty}^{\infty} \frac{Y \exp[-(Y-X)^2/4\theta]}{1+Y^2} dY \quad (C-2)$$

and are used to calculate the Doppler broadening effect on neutron cross sections. It is clear from the value of the integral of the exponential alone that

$$0 < \psi(x, 0) \leq 1 \quad ; \quad -1 < \chi(x, 0) < 1$$

Further

$$\psi(-x, 0) = \psi(x, 0) \quad ; \quad \chi(-x, 0) = -\chi(x, 0)$$

For each of the two functions two series are derived, one uniformly convergent and the other asymptotic. The selection of one of these two on the basis of speed and accuracy depends on the values of the arguments as described in the following discussion.

II. THE CALCULATION OF Ψ

A. CONVERGENT SERIES

The development of the uniformly convergent series for ψ is considered first. By writing the factor $\frac{1}{1+Y^2}$ as the Laplace transform of its inverse Laplace transform, we have

$$\psi(X, \theta) = \frac{1}{\sqrt{4\pi\theta}} \int_{-\infty}^{\infty} \exp\left[-(Y-X)^2/4\theta\right] dY \int_0^{\infty} \exp\left[-(1+Y^2)t\right] dt \quad (C-3)$$

Since the last integral converges uniformly, we may interchange the order of integration and then complete the square on Y . Thus,

$$\psi(X, \theta) = \frac{1}{\sqrt{4\pi\theta}} \int_0^{\infty} \exp\left[-t + \frac{X^2}{4\theta} \left(1 - \frac{1}{1+4\theta t}\right)\right] dt \int_{-\infty}^{\infty} \exp\left[-\left(\frac{1+4\theta t}{4\theta}\right) \left(Y - \frac{X}{1+4\theta t}\right)^2\right] dY \quad (C-4)$$

Now if

$$z = \left(\frac{1+4\theta t}{4\theta}\right)^{1/2} \left(Y - \frac{X}{1+4\theta t}\right) \quad (C-5)$$

$$\psi(X, \theta) = \int_0^{\infty} (1+4\theta t)^{-1/2} \exp\left[-t + \frac{X^2}{4\theta} - \frac{X^2}{(1+4\theta t)4\theta}\right] dt \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} e^{-z^2} dz \quad (C-6)$$

The last factor is unity. On changing the variable of integration to $u \equiv (1+4\theta t)/4\theta$, $\psi(X, \theta)$ may be expressed as

$$\begin{aligned} \psi(X, \theta) &= \exp\left[-(X^2-1)/4\theta\right] (4\theta)^{-1/2} \int_{1/4\theta}^{\infty} u^{-1/2} e^{-u} e^{\frac{1}{u} \left(\frac{X}{4\theta}\right)^2} du \\ &= (4\theta)^{-1/2} \left[\exp\left[-(X^2-1)/4\theta\right]\right] \int_{1/4\theta}^{\infty} e^{-u} u^{-1/2} \sum_{i=0}^{\infty} \frac{1}{i!} \left[\left(\frac{X}{4\theta}\right)^2 \frac{1}{u}\right]^i du \quad (C-7) \end{aligned}$$

Clearly the series may be integrated termwise. Define

$$\Gamma_0(\theta) = \frac{e^{1/4\theta}}{\sqrt{4\theta}} \int_{1/4\theta}^{\infty} u^{-1/2} e^{-u} du \quad (C-8)$$

$$\Gamma_i(\theta) = \frac{e^{1/4\theta}}{\sqrt{4\theta}} \int_{1/4\theta}^{\infty} u^{\frac{2i+1}{2}} e^{-u} du \quad (C-9)$$

Then

$$\Gamma_{i+1}(\theta) = \frac{2}{2i+1} \left[(4\theta)^i - \Gamma_i(\theta) \right] \quad (C-10)$$

and

$$\psi(X, \theta) = e^{\frac{X^2}{4\theta}} \sum_{i=0}^{\infty} \frac{1}{i!} \left(\frac{X}{4\theta} \right)^{2i} \Gamma_i(\theta) \quad (C-11)$$

The term $\Gamma_0(\theta)$ is tabulated using the extensive tables of the incomplete gamma function. With $\Gamma_0(X, \theta)$ and Equations (C-10) and (C-11), one may calculate $\psi(X, \theta)$ to any accuracy desired.

B. ASYMPTOTIC SERIES

To develop the asymptotic series we express $\psi(X, \theta)$ in slightly different form.

$$\psi = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-u^2}}{1 + (\lambda u + X)^2} du \quad (C-12)$$

where

$$\lambda = \sqrt{4\theta} \quad \text{and} \quad u = \frac{(Y-X)}{\sqrt{4\theta}}$$

and expand in a Taylor series with λ as argument. Thus,

$$\psi(X, \lambda) = \sum_{i=0}^{\infty} \frac{\lambda^i}{i!} \left. \frac{\partial^i \psi(X, \lambda)}{\partial \lambda^i} \right|_{\lambda=0} \quad (C-13)$$

Now the problem is to find

$$\left. \frac{\partial^i \psi(X, \lambda)}{\partial \lambda^i} \right|_{\lambda=0} \quad (C-14)$$

Clearly

$$\psi(X, 0) = \frac{1}{1+X^2} \quad (C-15)$$

Consider

$$\begin{aligned}
 F(X, \lambda) &= \frac{1}{1+(\lambda u+X)^2} = \frac{1}{u} \left[\frac{\frac{1}{u}}{\frac{1}{u^2} + \left(\lambda + \frac{X}{u}\right)^2} \right] \\
 &= \frac{1}{u} \int_0^\infty e^{-\left(\lambda + \frac{X}{u}\right)t} \sin \frac{t}{u} dt \\
 &= \int_0^\infty e^{-(u\lambda+X)z} \sin z dz
 \end{aligned} \tag{C-16}$$

where

$$z \equiv \frac{t}{u}$$

Then

$$\frac{\partial^i F}{\partial \lambda^i} = (-u)^i \int_0^\infty z^i e^{-(u\lambda+X)z} \sin z dz \tag{C-17}$$

and

$$\left. \frac{\partial^i \psi}{\partial \lambda^i} \right|_{\lambda=0} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^\infty (-u)^i e^{-u^2} du \int_0^\infty z^i e^{-Xz} \sin z dz \tag{C-18}$$

It is evident that for i odd

$$\left. \frac{\partial^i \psi(X, \lambda)}{\partial \lambda^i} \right|_{\lambda=0} = 0 \tag{C-19}$$

When i is even

$$\int_{-\infty}^\infty (-u)^i e^{-u^2} du = \left[\frac{\sqrt{\pi} \cdot 1 \cdot 3 \cdot 5 \cdots (i-1)}{2^i} \right] \tag{C-20}$$

and

$$\int_0^\infty z^i e^{-Xz} \sin z dz = \frac{\Gamma(i+1) \sin \left[(i+1) \sin^{-1} (1+X^2)^{-1/2} \right]}{(X^2+1) \frac{i+1}{2}} \tag{C-21}$$

Using the above results we may write

$$\psi(X, \theta) = \sum_{k=0}^{\infty} \left[\frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{2^k} \right] \frac{(4\theta)^k}{(X^2+1)^{\frac{2k+1}{2}}} \sin \left[(2k+1) \sin^{-1} (X^2+1)^{-1/2} \right] \quad (C-22)$$

The last series is asymptotic but will serve very well for some ranges of the parameters which complement the ranges over which (C-11) will converge rapidly.

III. THE CALCULATION OF CHI

By differentiating the integral form of $\psi(X, \theta)$ with respect to X , one determines that

$$\chi(X, \theta) = 2\theta \frac{\partial \psi}{\partial X} + X\psi \quad (C-23)$$

Then by differentiating the convergent series for $\psi(X, \theta)$ one obtains

$$\chi(X, \theta) = e^{-\frac{X^2}{4\theta}} \left(\frac{X}{4\theta}\right) \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{X}{4\theta}\right)^{2k} \Gamma_{k+1}(\theta) \quad (C-24)$$

Similarly by differentiating the asymptotic series for $\psi(X, \theta)$ one finds

$$\chi(X, \theta) = \sum_{k=0}^{\infty} \left| \frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{2^k} \right| \frac{(4\theta)^k}{(X^2+1)^{\frac{2k+1}{2}}} \cos \left[(2k+1) \sin^{-1} (X^2+1)^{-1/2} \right] \quad (C-25)$$

There is no need to calculate the trigonometric functions or the square root since

$$\begin{aligned} \frac{1}{\sqrt{X^2+1}} \sin \left[(2i+1) \sin^{-1} (X^2+1)^{-1/2} \right] &= \frac{1}{X^2+1} \text{ when } i = 0 \\ &= \frac{1}{\sqrt{X^2+1}} \left\{ \sin \left[(2i-1) \sin^{-1} (X^2+1)^{-1/2} \right] \frac{X^2}{X^2+1} \right. \\ &\quad \left. + \frac{2X}{X^2+1} \cos \left[(2i-1) \sin^{-1} (X^2+1)^{-1/2} \right] \right\} \\ &\text{when } i \neq 0 \end{aligned} \quad (C-26)$$

and

$$\begin{aligned} \frac{1}{\sqrt{X^2+1}} \left[\cos \left[(2i+1) \sin^{-1} (X^2+1)^{-1/2} \right] \right] &= \frac{X}{X^2+1} \text{ when } i = 0 \\ &= \frac{1}{\sqrt{X^2+1}} \left[\frac{X^2}{X^2+1} \cos \left[(2i-1) \sin^{-1} (X^2+1)^{-1/2} \right] \right. \\ &\quad \left. - \frac{2X}{X^2+1} \sin \left[(2i-1) \sin^{-1} (X^2+1)^{-1/2} \right] \right] \\ &\text{when } i \neq 0 \end{aligned} \quad (C-27)$$

Hence one may calculate Psi and Chi simultaneously by the asymptotic series.

IV. NUMERICAL PROCEDURE

The program uses the asymptotic series for values of X and θ for which it will give the accuracy desired and uses the convergent series elsewhere. The two regions are separated by a parabola whose coefficients must be determined experimentally. Moreover, a parabola which works for Ψ may be used for χ although the convergent series will be "overworked" in the latter case.

The convergent series are

$$\psi^a(X, \theta) = e^{-\frac{X^2}{4\theta}} \sum_{q=0}^Q \left(\frac{X}{4\theta}\right)^{2q} \alpha_q(4\theta) \quad (C-28)$$

where

$$\alpha_q(4\theta) = \frac{\Gamma_q(4\theta)}{q!} \quad (C-29)$$

$\Gamma_0(4\theta)$ is tabulated in a table of approximately 1200 values with its arguments, and

$$\Gamma_{q+1}(4\theta) = \frac{2}{2q+1} \left[(4\theta)^q \cdot \Gamma_q(4\theta) \right] \quad (C-30)$$

$$\chi^a(X, \theta) = \frac{X}{4\theta} e^{-\frac{X^2}{4\theta}} \sum_{q=0}^Q \left(\frac{X}{4\theta}\right)^{2q} \alpha'_q(4\theta) \quad (C-28a)$$

where

$$\alpha'_q(4\theta) = \frac{\Gamma_{q+1}(4\theta)}{q!} \quad (C-29a)$$

Q , the value of q at which the series (C-28) and (C-28a) are terminated, is defined as the value at which

$$\left\{ \left[\left(\frac{X}{4\theta}\right)^{2q} \alpha_q(4\theta) \right] / \sum_{q=0}^{Q-1} \left(\frac{X}{4\theta}\right)^{2q} \alpha_q(4\theta) \right\} \leq 0.0156 \quad (C-31)$$

The asymptotic series are

$$\psi^b(X, \theta) = \sum_{q=0}^4 \left[\frac{4\theta}{X^2+1} \right]^q \beta_q(X) \quad (C-32)$$

where

$$\beta_o(x) = \frac{1}{x^2+1} \quad (C-33)$$

$$\beta_1(x) = \frac{1}{2} \beta_o(x) [3-4 \beta_o(x)]$$

$$\beta_2(x) = \frac{3}{4} \beta_o(x) [5-20 \beta_o(x) + 16 \beta_o^2(x)]$$

$$\beta_3(x) = \frac{15}{8} \beta_o(x) [7-56 \beta_o(x) + 112 \beta_o^2(x) - 64 \beta_o^3(x)]$$

$$\beta_4(x) = \frac{105}{16} \beta_o(x) [9-120 \beta_o(x) + 432 \beta_o^2(x) - 576 \beta_o^3(x) + 256 \beta_o^4(x)] \quad (C-34)$$

$$\chi^b(x, \theta) = \sum_{q=0}^4 \left(\frac{4\theta}{x^2+1} \right)^q \beta_q'(x) \quad (C-32a)$$

where

$$\beta_o'(x) = \frac{x}{x^2+1} \quad (C-33a)$$

$$\beta_1'(x) = -\frac{1}{2} \beta_o'(x) [3-4x \beta_o'(x)]$$

$$\beta_2'(x) = \frac{3}{4} \beta_o'(x) [5-20x \beta_o'(x) + 16x^2 \beta_o'^2(x)]$$

$$\beta_3'(x) = -\frac{15}{8} \beta_o'(x) [7-56x \beta_o'(x) + 112x^2 \beta_o'^2(x) - 64x^3 \beta_o'^3(x)]$$

$$\begin{aligned} \beta_4'(x) = \frac{105}{16} \beta_o'(x) [9-120x \beta_o'(x) + 432x^2 \beta_o'^2(x) \\ - 576x^3 \beta_o'^3(x) + 256x^4 \beta_o'^4(x)] \end{aligned} \quad (C-34a)$$

The conditions under which ψ^a is used are:

$0 \leq x < 1.2$	and	$4\theta \geq 0.275 x^2 + 0.05$
$1.2 \leq x < 10$	and	$4\theta \geq 0.12 x^2 + 0.28$
$10 \leq x < 100$	and	$4\theta \geq 0.105 x^2 + 1.75$
$100 \leq x < 200$	and	$4\theta \geq 0.095 x^2 + 100$

APPENDIX D RESONANCE EQUATIONS

The single level Breit-Wigner formula for the scattering and radiative capture cross sections near a resonance are

$$\sigma_s(E') = \pi \kappa_o^2 g \left[\frac{\Gamma_n^2 + \frac{2\Gamma_n}{\kappa_o \sqrt{\pi}} (E' - E_o) \sqrt{\sigma_p}}{(E' - E_o)^2 + (\Gamma/2)^2} \right] + \sigma_p$$

$$\sigma_c(E') = \pi \kappa_o \kappa g \frac{\Gamma_n \Gamma \gamma}{(E' - E_o)^2 + (\Gamma/2)^2} \quad (D-1)$$

where E' is the energy in the center of mass system, κ_o is the reduced wave length in the center of mass system corresponding to energy E_o , and R is the effective radius of the nucleus. The energy in the center of mass system is the sum of the energies of the neutron and nucleus obtained using their center of mass system velocities.

$$E' = \frac{1}{2} \frac{mM}{m+M} \left| \vec{v} - \vec{V} \right|^2 \quad (D-2)$$

where m is the neutron mass, M the nuclear mass and $\vec{v}$ and $\vec{V}$ their respective laboratory system velocities.

$$E' = \left[E + \frac{m}{M} E_N - v_p \sqrt{2mE} \right] \frac{M}{m+M} \quad (D-3)$$

where E is the laboratory system neutron energy, E_N that of the nucleus, and v_p is the component of the velocity of the nucleus parallel to that of the neutron.

Neglecting the second term in (D-3)

$$v_p \approx \frac{E - \frac{m+M}{M} E'}{\sqrt{2mE}}$$

$$dv_p \approx - \frac{m+M}{M} \frac{1}{\sqrt{2mE}} dE' \quad (D-4)$$

Assuming a Maxwellian distribution of velocities for the nuclei, the probability of a particular value of v_p is

$$\begin{aligned}
P(v_p) dv_p &= \sqrt{\frac{M}{2\pi KT}} \exp \left[-\frac{Mv_p^2}{2kT} \right] dv_p \\
&= \sqrt{\frac{M}{2\pi KT}} \exp \left[-\frac{M}{2KT} \left(E - \frac{m+M}{M} E' \right)^2 / 2mE \right] \frac{M+m}{M\sqrt{2mE}} dE' \\
&\equiv P(E':E) dE'
\end{aligned} \tag{D-5}$$

The effective Doppler broadened cross section, $\sigma_D(E)$, is that for which $v \sigma_D(E)$ is equal to the actual reaction rate.

$$\begin{aligned}
\sigma_D(E) &= \frac{1}{v} \int_0^\infty P(E':E) \sigma(E') \left| \vec{v} - \vec{V} \right| dE' \\
&= \int_0^\infty P(E':E) \sigma(E') \sqrt{\frac{M+m}{M} \frac{E'}{E}} dE'
\end{aligned} \tag{D-6}$$

$$\begin{aligned}
\sigma_{D_\gamma}(E) &= \int_0^\infty \sqrt{\frac{M}{4\pi KT E}} \left(\frac{M+m}{M} \right) \exp \left[-\frac{M}{2KT} \left(E - \frac{m+M}{M} E' \right)^2 / 2mE \right] \\
&\quad \left[\frac{\pi h^2}{2 \frac{mM}{m+M} \sqrt{E_0 E'}} g \frac{\Gamma_n \Gamma_\gamma}{(E' - E_0)^2 + (\Gamma/2)^2} \left(\frac{m+M}{M} \right)^{1/2} \left(\frac{E'}{E} \right)^{1/2} \right] dE'
\end{aligned} \tag{D-7}$$

$$\text{let } X = \left[\frac{M}{m+M} E - E_0 \right] / \Gamma/2, \quad Y = \left[E' - E_0 \right] / \Gamma/2$$

$$\theta = \frac{4mEKT}{M\Gamma^2} \left(\frac{M}{m+M} \right)^2 \tag{D-8}$$

Then

$$\begin{aligned}
\sigma_{D_\gamma}(E) &= \frac{1}{\sqrt{4\pi\theta}} \frac{4\pi h^2}{2mE_0} g \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} \left(\frac{m+M}{M} \right)^{3/2} \left(\frac{E_0}{E} \right)^{1/2} \\
&\quad \int_{-\frac{2E_0}{\Gamma}}^\infty \frac{\exp[-(X-Y)^2/4\theta]}{1+Y^2} dY
\end{aligned} \tag{D-9}$$

Only values of Y close to X contribute significantly to the integral in (D-9); since values of X near $-\frac{2E_0}{\Gamma}$ occur only for E near zero and since θ is proportional to E only a negligible error is introduced by extending the lower limit to $-\infty$. Thus, defining

$$\sigma_{\gamma_0} \equiv \frac{4\pi \hbar^2}{2mE_0} g \left(\frac{m+M}{M}\right)^{3/2} \left(\frac{E_0}{E}\right)^{1/2} \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} \quad (D-10)$$

and

$$\psi \equiv \frac{1}{\sqrt{4\pi\theta}} \int_{-\infty}^{\infty} \frac{\exp[-(X-Y)^2/4\theta]}{1+Y^2} dY \quad (D-11)$$

$$\sigma_{D_\gamma} \approx \sigma_{\gamma_0} \psi(X, \theta) \quad (D-12)$$

Similarly

$$\sigma_{D_s}(E) = \frac{1}{\sqrt{4\pi\theta}} \frac{4\pi \hbar^2}{2mE_0} g \frac{\Gamma_n^2}{\Gamma^2} \left(\frac{m+M}{M}\right)^{3/2} \int_{-\infty}^{\infty} \frac{\exp[-(X-Y)^2/4\theta] \left[1 + \frac{\Gamma \sqrt{\sigma_p}}{\chi_0 \Gamma_n \sqrt{\pi}} Y\right]}{1+Y^2} \left(\frac{E'}{E}\right)^{1/2} + \sigma_p \quad (D-13)$$

The factor $\left(\frac{E'}{E}\right)^{1/2}$ may be expanded as

$$\begin{aligned} \left(\frac{E'}{E}\right)^{1/2} &= \left[\frac{\Gamma}{2E} (Y-X) + \frac{M}{m+M} \right]^{1/2} \\ &\approx \left(\frac{M}{m+M}\right)^{1/2} \left[1 + \frac{m+M}{M} \frac{\Gamma}{4E} (Y-X) + \dots \right] \end{aligned} \quad (D-14)$$

over the significant portion of the range of Y.

For all cases of interest this is adequately approximated by $\left(\frac{M}{m+M}\right)^{1/2}$

Defining

$$\sigma_{s_0} \equiv \frac{4\pi \hbar^2}{2mE_0} g \left(\frac{m+M}{M}\right)^2 \frac{\Gamma_n^2}{\Gamma^2} \quad (D-15)$$

and

$$\chi(X, \theta) \equiv \frac{1}{\sqrt{4\pi\theta}} \int_{-\infty}^{\infty} \frac{Y \exp[-(X-Y)^2/4\theta]}{1+Y^2} dY \quad (D-16)$$

$$\sigma_{D_s} = \sigma_{s_o} \psi(X, \theta) + 2 \frac{m+M}{M} \sqrt{g \sigma_p \sigma_{s_o}} \chi(X, \theta) + \sigma_p \quad (D-17)$$

The process of locating the central energies of unresolved resonances described in the main portion of this report assumes a constant density of resonances. In reality there are two phenomena which cause the level density to vary. One is the variation in the density of nuclear levels of zero angular momentum, the second is the appearance of higher angular momentum levels. Present information indicates the plausibility of the expression

$$D = D_o \exp - \left[\sqrt{B E^*} \right] \quad (D-18)$$

$$B = 4.8 \times 10^{-5} \text{ ev}^{-1}$$

for the average spacing between levels as a function of E^* , the excitation energy of the compound nucleus. For isotopes of atomic weight in the vicinity of that of uranium, E^* is approximately equal to the incident energy of the neutron plus 6 MEV. Thus in the energy range in which the resonance function cross sections will be used in RBU, E^* is not a strong function of V , the neutron velocity. Equation (D-18) may then be conveniently approximated by

$$D_o e^{-\sqrt{6 \times 10^6 B} \left(1 - \frac{E}{2 \sqrt{6 \times 10^6 B}} \right)} \quad (D-19)$$

A rough approximation to the effect of resonances of angular momentum higher than zero can be obtained by the classical treatment of glancing collisions according to which the highest angular momentum which can contribute to an interaction between a neutron and a nucleus is given by

$$\ell_{\max} = m v R / \hbar \quad (D-20)$$

where R is the radius of the nucleus given approximately by $1.45 \times 10^{-13} A^{1/3}$ cm. If one assumes that all angular momenta capable, according to (D-20) of contributing to interactions, produce effectively similar resonances, it appears reasonable to write that the effective density of resonances is given by

$$\frac{1}{D} = \frac{1}{D_o} \left(1.45 \times 10^{-13} A^{1/3} m v / \hbar + 1 \right) \quad (D-21)$$

The effect of higher angular momentum resonances, like the effect of the variation of nuclear level density is small enough that these rough approximations are probably satisfactory for reactor calculations but large enough that they should be included. In RBU, the fact that the most significant property of the resonances is the average cross section, the product of the level density and the mean cross section within a resonance leads to one further approximation. The variation in level density given by (D-18) and (D-21) is treated as a variation in the cross section value and the level density is treated as a constant. One source of error associated with this approximation arises from the fact that the effect of cross section value variation is diminished by self-shielding while that of level density variation is not. It appears, however, in view of the small importance of the two phenomena considered here, that the approximate treatment is sufficient.

APPENDIX E
DERIVATION OF THE BACKWARD DIFFERENCE EQUATIONS

For a time interval, δ , the backward differences of N are defined by

$$\begin{aligned}\nabla^0(t) &= \dot{N}(t) \\ \nabla^r(t) &= \nabla^{r-1}(t) - \nabla^{r-1}(t-\delta)\end{aligned}\quad (E-1)$$

Equations (E-1) may be solved for the values of $\dot{N}$ at preceding time steps:

$$\begin{aligned}\dot{N}(t) &= \nabla^0(t) \\ \dot{N}(t-\delta) &= \nabla^0(t) - \nabla^1(t) \\ \dot{N}(t-n\delta) &= \sum_{r=0}^n (-1)^r \binom{n}{r} \nabla^r(t)\end{aligned}\quad (E-2)$$

Equation (E-2) yields values of N at one point for each of the R backward differences available. The value of $\dot{N}$ at an arbitrary time, t' , may then be approximated by a power series

$$\dot{N}(t') = \sum_{r=0}^R A_r (t' - t)^r \quad (E-3)$$

Combining Equations (E-2) and (E-3), one obtains a set of R simultaneous algebraic equations in the A_r

$$\sum_{r=0}^R A_r (n\delta)^r = \sum_{i=0}^n (-1)^i \binom{n}{i} \nabla^i(t) \quad (E-4)$$

For a given value of R , these may be solved by elimination to give

$$\begin{aligned}A_1 &= \frac{1}{\delta} \left[\nabla^1 + \frac{1}{2} \nabla^2 + \frac{1}{3} \nabla^3 + \frac{1}{4} \nabla^4 + \frac{1}{5} \nabla^5 + \dots \right] \\ A_2 &= \frac{1}{\delta^2} \left[\frac{1}{2} \nabla^2 + \frac{1}{2} \nabla^3 + \frac{11}{24} \nabla^4 + \frac{5}{12} \nabla^5 + \dots \right] \\ A_3 &= \frac{1}{\delta^3} \left[\frac{1}{6} \nabla^3 + \frac{1}{4} \nabla^4 + \frac{7}{24} \nabla^5 + \dots \right] \\ A_4 &= \frac{1}{\delta^4} \left[\frac{1}{24} \nabla^4 + \frac{1}{12} \nabla^5 + \dots \right] \\ A_5 &= \frac{1}{\delta^5} \left[\frac{1}{120} \nabla^5 + \dots \right] \\ &\text{et cetera}\end{aligned}\quad (E-5)$$

For smaller values of R the same solutions hold if the ∇^r for $r > R$ are set equal to zero.

By substituting the appropriate values of t' in (E-3) and using the coefficients of (E-5) for $R=3$, the interpolation equation for $\dot{N}$ given in the main body of this report is obtained. Similarly by integrating (E-3) and making the same substitution the prediction and correction formulae are found.

APPENDIX F
DERIVATION OF THE DIFFUSION DIFFERENCE EQUATIONS

The diffusion equation in one dimension is

$$f(r) = - \frac{1}{r^\rho} \frac{\partial}{\partial r} D(r) r^\rho \frac{\partial}{\partial r} \phi(r) + T(r) \phi(r) - H(r) = 0 \quad (F-1)$$

To obtain an equation involving values of the neutron flux at the mesh points $r=r_0, r_1 \dots r_N$ only, one multiplies Equation (F-1) by r^ρ and integrates from

$$\frac{r_{n-1} + r_n}{2} \equiv r_{n-1/2} \quad \text{to} \quad \frac{r_n + r_{n+1}}{2} \equiv r_{n+1/2} \quad (F-2)$$

Between $r_{n-1/2}$ and r_n and between r_n and $r_{n+1/2}$, the nuclear constants, D and T , do not vary. Then assuming that ϕ and H vary linearly between mesh points:

$$\begin{aligned} \int_{r_{n-1/2}}^{r_{n+1/2}} r^\rho f(r) dr &= - D_{n-} r^\rho \frac{\partial}{\partial r} \phi(r) \Big|_{r_{n-1/2}}^{r_n} - D_{n+} r^\rho \frac{\partial}{\partial r} \phi(r) \Big|_{r_n}^{r_{n+1/2}} \\ &+ T_{n-} \int_{r_{n-1/2}}^{r_n} r^\rho \left[\phi_n + \frac{\phi_n - \phi_{n-1}}{\Delta r_{n-}} (r - r_n) \right] dr \\ &+ T_{n+} \int_{r_n}^{r_{n+1/2}} r^\rho \left[\phi_n + \frac{\phi_{n+1} - \phi_n}{\Delta r_{n+}} (r - r_n) \right] dr \\ &- \int_{r_{n-1/2}}^{r_n} r^\rho \left[H_{n-} + \frac{H_{n-} - H_{n-1}}{\Delta r_{n-}} (r - r_n) \right] dr \\ &- \int_{r_n}^{r_{n+1/2}} r^\rho \left[H_{n+} + \frac{H_{n+1} - H_{n+}}{\Delta r_{n+}} (r - r_n) \right] dr = 0 \end{aligned} \quad (F-3)$$

In (F-3) $H(r)$ is permitted to be discontinuous at mesh points while ϕ has been assumed to be continuous.

$$\begin{aligned}
\int_{r_{n-1/2}}^{r_{n+1/2}} r^\rho f(r) dr = & - D_{n-} \frac{\phi_n - \phi_{n-1}}{\Delta r_{n-}} \left[r_n^\rho - \left(r_n - \frac{1}{2} \Delta r_{n-} \right)^\rho \right] \\
& - D_{n+} \frac{\phi_{n+1} - \phi_n}{\Delta r_{n+}} \left[\left(r_n + \frac{1}{2} \Delta r_{n+} \right)^\rho - r_n^\rho \right] \\
& + T_{n-} \left[\frac{1}{\rho+1} r^{\rho+1} \phi_n + \frac{\phi_n - \phi_{n-1}}{\Delta r_{n-}} \left(\frac{1}{\rho+2} r^{\rho+2} - \frac{1}{\rho+1} r_n r^{\rho+1} \right) \right]_{r_{n-1/2}}^{r_n} \\
& + T_{n+} \left[\frac{1}{\rho+1} r^{\rho+1} \phi_n + \frac{\phi_{n+1} - \phi_n}{\Delta r_{n+}} \left(\frac{1}{\rho+2} r^{\rho+2} - \frac{1}{\rho+1} r_n r^{\rho+1} \right) \right]_{r_n}^{r_{n+1/2}} \\
& - \left[H_{n-} \frac{1}{\rho+1} r^{\rho+1} + \frac{H_{n-} - H_{n-1+}}{\Delta r_{n-}} \left(\frac{1}{\rho+2} r^{\rho+2} - \frac{1}{\rho+1} r_n r^{\rho+1} \right) \right]_{r_{n-1/2}}^{r_n} \\
& - \left[H_{n+} \frac{1}{\rho+1} r^{\rho+1} + \frac{H_{n+1} - H_{n+}}{\Delta r_{n+}} \left(\frac{1}{\rho+2} r^{\rho+2} - \frac{1}{\rho+1} r_n r^{\rho+1} \right) \right]_{r_n}^{r_{n+1/2}} = 0 \quad (F-4)
\end{aligned}$$

On substituting limits and collecting terms, one finds

$$-a_n \phi_{n-1} + b_n \phi_n - c_n \phi_{n+1} + a'_n H_{n-1+} - b'_n H_{n-} - b''_n H_{n+} + c'_n H_{n+1} = 0$$

$$a_n = D_{n-} \frac{r_{n-1/2}}{\Delta r_{n-}} + T_{n-} a'_n$$

$$b_n = a_n + c_n + T_{n-} \frac{r_n^{\rho+1} - r_{n-1/2}^{\rho+1}}{(\rho+1)} - T_{n+} \frac{r_n^{\rho+1} - r_{n+1/2}^{\rho+1}}{\rho+1}$$

$$c_n = \frac{r_{n+1/2}^\rho}{\Delta r_{n+}} + T_{n+} c'_n$$

$$a'_n = \frac{r_n^{\rho+2} - r_{n-1/2}^{\rho+2}}{\rho+2 \Delta r_{n-}} - \frac{r_n^{\rho+2} - r_n r_{n-1/2}^{\rho+1}}{(\rho+1) \Delta r_{n-}}$$

$$c'_n = \frac{r_n^{\rho+2} - r_{n+1/2}^{\rho+2}}{(\rho+2) \Delta r_{n+}} - \frac{r_n^{\rho+2} - r_n r_{n+1/2}^{\rho+1}}{(\rho+1) \Delta r_{n+}} \quad (F-5)$$

$$b'_n = a'_n + \frac{r_n^{\rho+1} - r_{n-1/2}^{\rho+1}}{\rho+1}$$

$$b''_n = c'_n - \frac{r_n^{\rho+1} - r_{n+1/2}^{\rho+1}}{\rho+1} \quad (F-5)$$

The approximation

$$r_n^\rho - r_{n-1/2}^\rho \approx \frac{1}{2} \rho r_n^{\rho-1} \Delta r_{n-} \quad (F-6)$$

is accurate to first order in Δr . With this approximation

$$a'_n = c'_n = 0$$

and (F-5) reduces to

$$-a_n \phi_{n-1} + b_n \phi_n - c_n \phi_{n+1} - d_{n-} H_{n-} - d_{n+} H_{n+} = 0$$

where

$$a_n = (D_{n-}) \frac{r_{n-1/2}^\rho}{\Delta r_{n-}}$$

$$b_n = a_n + c_n - T_n - r_n^\rho \frac{\Delta r_{n-}}{2} - T_{n+} r_n^\rho \frac{\Delta r_{n+}}{2}$$

$$c_n = (D_{n+}) \frac{r_{n+1/2}^\rho}{\Delta r_{n+}}$$

$$d_{n-} = r_n^\rho \frac{\Delta r_{n-}}{2}, \quad d_{n+} = r_n^\rho \frac{\Delta r_{n+}}{2}$$

APPENDIX G DERIVATION OF THE EQUATION FOR THE DIFFUSION COEFFICIENT

The diffusion coefficient is defined as the quantity which, when multiplied by the component of the gradient of the neutron flux density normal to a surface, gives the current across that surface

$$D \hat{n} \cdot \vec{\nabla} \phi = J_n \quad (G-1)$$

The diffusion coefficient in RBU, then, is to be computed from

$$D = \frac{\int_S \vec{J} \cdot \hat{n} \, ds}{\int_S \hat{n} \cdot \vec{\nabla} \phi \, ds} \quad (G-2)$$

where ds is an element of area of the surface bounding a region.

The numerator of this expression is obtained simply by tallying the leakage out of the region in question. The expectation value of the contribution made by a neutron to the normal component of the gradient of the flux density at a surface may be obtained as follows.

Consider the neutron to start at point x, y, z , moving in a direction α, β, γ with velocity, such that the mean free path is λ , toward a boundary surface, S , whose locus is

$$A(x-x_0)^2 + B(y-y_0)^2 + C(z-z_0)^2 - K = 0 \quad (G-3)$$

Construct two additional surfaces, S' and S'' which differ only in that

$$\begin{aligned} K' &= K - \epsilon \\ \text{and} \quad K'' &= K + \epsilon \end{aligned} \quad (G-4)$$

where ϵ is a small distance. The three surfaces define two regions, 1 and 2, and the distances the neutron must travel to reach each of these boundaries are

$$\begin{aligned} s' &= \frac{-e + g \sqrt{e^2 - hr'}}{h} \\ s &= \frac{-e + g \sqrt{e^2 - hr}}{h} \end{aligned}$$

$$S'' = \frac{-e+g\sqrt{e^2-hr''}}{h}$$

where

$$e = A\alpha(x-x_0) + \beta(y-y_0) + C\gamma(z-z_0)$$

$$h = A\alpha^2 + B\beta^2 + C\gamma^2$$

$$r = A(x-x_0)^2 + B(y-y_0)^2 + C(z-z_0)^2 - K$$

$$r' = r + \epsilon$$

$$r'' = r - \epsilon$$

(G-5)

The distances the particle will have to travel to cross each of the regions are

$$S_1 = S - S' = \frac{g}{h} \left[\sqrt{e^2 - hr} - \sqrt{e^2 - hr'} \right]$$

$$\approx \frac{g}{2} \frac{\epsilon}{(e^2 - hr)^{1/2}} + \frac{g}{8} \frac{\epsilon^2 h}{(e^2 - hr)^{3/2}} - \mathcal{O}(\epsilon^3)$$

$$S_2 = S'' - S = \frac{g}{h} \left[\sqrt{e^2 - hr''} - \sqrt{e^2 - hr'} \right]$$

$$\approx \frac{g}{2} \frac{\epsilon}{(e^2 - hr)^{1/2}} - \frac{g}{8} \frac{\epsilon^2 h}{(e^2 - hr)^{3/2}} - \mathcal{O}(\epsilon^3)$$

(G-6)

The expectation values of the contribution to the the neutron flux densities in each of the two small regions are

$$\phi_1 = \lambda e^{-S'/\lambda} \left(\frac{1 - e^{-S_1/\lambda}}{1 - e^{-S'/\lambda}} \right) / V_1$$

$$\phi_2 = \lambda e^{-S/\lambda} \left(\frac{1 - e^{-S_2/\lambda}}{1 - e^{-S/\lambda}} \right) / V_2$$

(G-7)

where V_1 and V_2 are the volumes per unit surface area; they may be represented as the product of ϵ with a constant, L , in each region. Since ϵ and, therefore, S_1 and S_2 are small

$$\phi_1 = \lambda e^{-S/\lambda} \left(\frac{e^{S_1/\lambda} - 1}{e^{S'/\lambda} - 1} \right) / L\epsilon$$

$$\approx \frac{1}{L\epsilon} \lambda e^{-S/\lambda} \left[\frac{S_1}{\lambda} + \frac{1}{2} \left(\frac{S_1}{\lambda} \right)^2 + \mathcal{O} \left(\frac{S_1^3}{\lambda^3} \right) \right]$$

(G-8)

$$\phi_2 \approx \frac{1}{L\epsilon} \lambda e^{-S/\lambda} \left[\frac{s_2}{\lambda} - \frac{1}{2} \left(\frac{s_2}{\lambda} \right)^2 + \theta \left(\frac{s_2}{\lambda} \right)^3 \right] \quad (G-8)$$

The derivative of the contribution to the neutron flux with respect to distance S along the path of motion is

$$\begin{aligned} \frac{\partial \phi}{\partial S} &= \lim_{\epsilon \rightarrow 0} \frac{\phi_2 - \phi_1}{\frac{1}{2} (S_1 + S_2)} \\ &= \frac{1}{2L} e^{-S/\lambda} \left[g \frac{h}{(e^2 - hr)} - \frac{1}{\lambda} \frac{1}{(e^2 - hr)^{1/2}} \right] \end{aligned} \quad (G-9)$$

The constant L is equal to the normal distance between surfaces per unit ϵ which, from Equation (G-6) is

$$L \approx \frac{g}{2(e^2 - hr)^{1/2}} \nabla$$

where ∇ is the cosine of the angle between the direction of motion of the particle and the normal to the surface. Substituting this expression for L and dividing by ∇ , we obtain the contribution to the normal component of the gradient of the flux

$$\frac{\partial \phi}{\partial n} = \frac{e^{-S/\lambda}}{\nabla^2} \left[\frac{g h}{(e^2 - hr)^{1/2}} - \frac{1}{\lambda} \right] \quad (G-10)$$

It is interesting to note that the quantity $(e^2 - hr)$ in this expression is independent of the position along the particle's path at which it is computed.