DP - 446

Physics and Mathematics

AEC Research and Development Report

A MONTE CARLO CODE FOR THE TRANSPORT OF NEUTRONS

by

W. V. Baxter

Theoretical Physics Division

December 1959

E. I. du Pont de Nemours & Co.
Savannah River Laboratory
Aiken, South Carolina

Printed in USA. Price $1.00
Available from the Office of Technical Services
U. S. Department of Commerce
Washington 25, D. C.

255289

DP - 446

PHYSICS AND MATHEMATICS
(TID-4500, 15th Ed.)

A MONTE CARLO CODE FOR THE TRANSPORT OF NEUTRONS

by

William V. Baxter

December 1959

E. I. du Pont de Nemours & Co.
Explosives Department - Atomic Energy Division
Technical Division - Savannah River Laboratory

Printed for
The United States Atomic Energy Commission
Contract AT(07-2)-1

Approved by
D. S. St. John, Research Manager
Theoretical Physics Division

ABSTRACT

A Monte Carlo code for the IBM 704 computer was written to study the transport of neutrons in a uniform heterogeneous lattice of cylindrical fuel assemblies. Models of the geometric and physical processes are used to obtain the neutron age and migration area; the flux as a function of position, energy, and direction; and absorption data from which thermal utilization and the multiplication constant k_∞ may be calculated.

CONTENTS

LIST OF FIGURES

A MONTE CARLO CODE FOR THE TRANSPORT OF NEUTRONS

INTRODUCTION

A computer code was needed at the Savannah River Laboratory to calculate the space-energy distribution of the neutron flux, the migration area, and the absorption in a heterogeneous reactor lattice. Such parameters are used in reactor design to predict the performance of untested fuel components.

The reactor lattice parameters have been obtained at SRL from calculations for a lattice cell by means of the group diffusion method[1], or the P_3 approximation[2] in one group. In strongly absorbing fuel assemblies, however, the former method does not yield a good representation of the local anisotropies in the neutron flux, while the latter method does not permit one to account for spectral hardening. To overcome these deficiencies, the Monte Carlo method was chosen, since it allows a detailed study of the spatial flux at all energies from fission to thermal.

Although the Monte Carlo method has been applied to neutron transport studies before,[4,5] no single computer program could be applied directly to the problems of interest at SRL. However, the logic in portions of several of these programs was directly applicable to the program described in this report. For example, the logic of Cashwell[3] was used to determine the neutron location within the basic lattice cell, and the logic of Brown[6] was used for the collision mechanics.

This report describes an IBM 704 computer code that has been written to study the slowing down of neutrons in an infinite lattice of cylindrical fuel assemblies. The code will treat problems involving a variable number of geometrical regions and isotopic mixtures. The results obtained when this code is used in the study of particular lattices will be published separately.

SUMMARY

A Monte Carlo code was prepared for the IBM 704 computer to study the transport of neutrons in a heterogeneous lattice of cylindrical fuel assemblies. The code assumes a uniform lattice of fuel elements made up of concentric cylindrical regions and situated at centers of rectangles in an infinite array. A fuel assembly, with its associated coolant, cladding, and housings, may be composed of as many as 12 concentric regions. Each region contains one of five possible mixtures of isotopes.

The code, Casino 13, is made up of various subroutines, including source, geometry, direction cosines, scattering, and collision mechanics. IBM Share Library routines for input and output control and standard mathematical functions are used. The subroutines for generating

neutron histories are assembled by the SAP 3 Compiler[17] along with analysis and editing routines, which develop and print out summaries of the collision data. The subroutines are for the most part independent so that a variety of problems may be handled by reassembling the subroutines as needed with some extra coding.

An auxiliary routine is used to generate an input cross section tape for Casino 13. Tables of microscopic cross sections, containing a number of entries that may be different for each element, are expanded by a logarithmic interpolation formula into tables of 128 values each. These values are then multiplied by the number of nuclei per unit volume to give macroscopic values, which are combined to give total cross sections for each isotopic mixture. Machine time of 5 minutes is required to generate a cross section tape.

Neutrons are processed 300 at a time through each of three energy bands, with individual histories being preserved from one band to the next. The use of energy bands was necessary because of the storage limitation of 16,384 words on the IBM 704 at NYU at the time the code was written. A complete sample, or "batch", consists of 600 neutrons, as determined by a 50-value fission spectrum and 12 initial directions for each fission energy. Absorption by region, migration area, and the neutron age are printed at the end of each batch. Flux data are printed at the end of each run, which consists of any desired number of batches. Running time is approximately 35 minutes per batch for a nine-region problem.

DISCUSSION

CASINO 13 CODE

A Monte Carlo code for the IBM 704 computer is used at the Savannah River Laboratory to study the slowing down of neutrons in an infinite heterogeneous lattice of concentric cylindrical fuel assemblies. Neutrons are started at fission energies, and their histories are computed as they undergo elastic collisions until thermalization and eventual termination occur. At each collision a scattering mass is determined according to the relative cross sections at the neutron's energy and in the isotopic mixture in which the collision occurs. Current values of the location coordinates, the geometrical region, and the mixture index are kept throughout the calculation of each neutron history. A weight parameter, initially equal to 1, is used for tabulating absorption data at each collision and for deciding when "Russian roulette" should be played for terminating the neutron*.

Scattering is assumed to be isotropic in the center-of-mass frame of reference at all energies, and isotropic in the laboratory system for

* The method used in playing "Russian roulette" is discussed under Weighting Procedure, page 11.

energies above 1 ev. The energy loss and the cosine of the laboratory scattering angle are determined from the equations of elastic collision. Three-dimensional direction cosines (λ_1,μ_1,ν_1) are determined by a random rotation after scattering of a neutron through an angle ω, in the laboratory system, from an incident direction (λ,μ,ν).

Computing time is reduced by using stored tables for trigonometric functions and logarithms. A simple random number system is employed, and the use of square root is avoided whenever possible in the geometry routine.

At each collision a tabulation of the directional flux is obtained in 1 of 18 energy ranges and in 1 of 32 space-volume elements. A contribution to the migration area is computed at each collision, and an addition to the Fermi age is made if the neutron energy drops below E_K for the first time. Absorption by region for thermal and epithermal energies is noted throughout the calculation.

The order in which the different phases of the calculation are performed is shown in Flowsheet 1, and in the discussion that follows the various subroutines are presented as nearly as possible in their normal order of application.

SOURCE

Neutron histories are initiated by the source routine, which assigns a fission energy and a set of direction cosines to each neutron. In addition, 2700 storages are initialized with the neutron name, the location coordinates of the source, and an initial weight. Each name is a composite word containing the indices of the batch, neutron, collision, region, and isotopic mixture. The 2700 storages are used to preserve neutron data in order that 300 neutrons may be processed through one energy band and then resumed in the next lower energy band.

A table of 50 fission energies is used sequentially, and 12 neutrons per batch are started with each energy. Because of storage limitations neutrons are processed in sets of 300 each, with two sets making up a batch, or complete sample. The lower half of the fission energy spectrum is used with the first set, and the remainder is used to complete the batch.

The fission spectrum was obtained by stepwise integration of the function

$$\sqrt{E}\ \exp\ (-0.775E)dE$$

in the limits from 0 to ∞. Energies obtained correspond to internal points of energy intervals, the bounds of which divide the total integral into 50 equal parts. The integration was performed using a Newton-Raphson procedure.

Neutrons are emitted initially from the surface of a point sphere at a point in a fuel region on either the x or the y axis. A schematic diagram of a fuel element with cylindrical geometry is shown in Figure 1. From symmetry considerations it is necessary that the initial directions of travel of the neutrons be chosen only from one quadrant of the sphere. For example, if the source is on the x axis, the directions are chosen from the first quadrant. Instead of using a completely isotropic source in the laboratory system, a device is employed that assures a nearly uniform distribution of initial directions while using only a small sample. An octant of a sphere is divided into six spherical triangles of equal area by drawing the medians from each of its vertices. If an octant is divided in this manner, the direction cosines of a radius vector in each of the triangles have a definite permutation relative to magnitude. The initial direction cosines, (λ,μ,ν), are picked at random, ordered according to magnitude, and then assigned by permutation to one of the six triangles. Of the 12 neutrons born at each fission energy, 6 have all positive direction cosines, so that one neutron trajectory is assigned to each triangle in the first octant. The remaining 6 sets are formed in an identical manner, and then a negative sign is affixed to either λ or μ depending on whether the source is on the x or y axis.

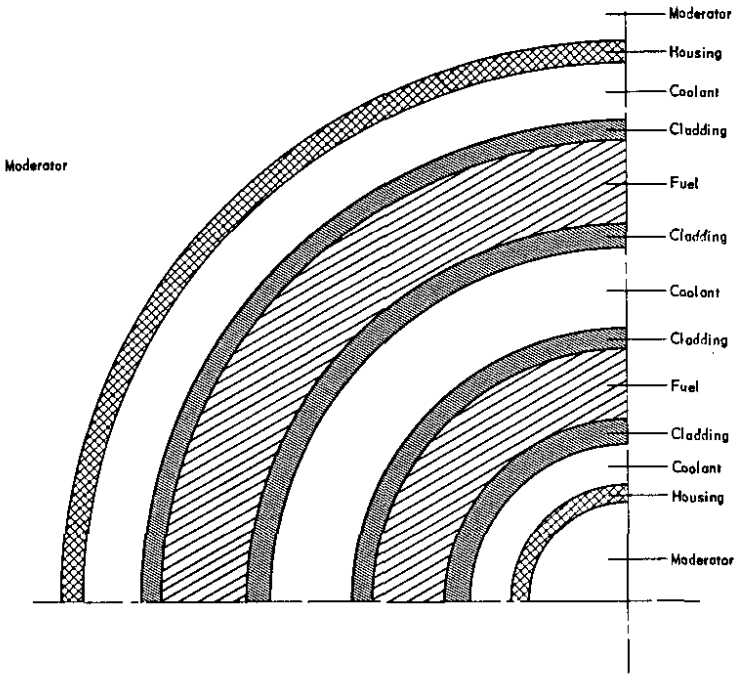


FIGURE 1 – FUEL ELEMENT WITH CYLINDRICAL GEOMETRY

The method of selecting direction cosines for the source neutrons is as follows. In a spherical coordinate system the radius vector has direction coordinates given by the formulas

$$\lambda = \sin \omega \cos \Phi$$

$$\mu = \sin \omega \sin \Phi$$

$$\nu = \cos \omega$$

where ω is a polar angle and Φ is azimuthal. By means of a random number, r, in the interval $0 \leq r < 1$, the source routine picks cos Φ from a table of values corresponding to values of Φ distributed uniformly from 0 to $\frac{\pi}{2}$. The same table is used to determine sin Φ, since sin Φ is equal to cos $(\frac{\pi}{2} - \Phi)$. Cos ω is uniformly distributed from 0 to 1. The value of sin ω, equal to $(1 - \cos^2\omega)^{\frac{1}{2}}$, is obtained from a table.

RANDOM NUMBERS

Two random number chains are used so that if two problems are run with different input parameters, corresponding neutrons in each problem can be started with the same random number. The first of these pseudo-random number sequences is generated by the congruence formula

$$r_{n+1} \equiv 3^{21} r_n \pmod{2^{35}}$$

and the second is formed by the relation

$$r_{n+1} \equiv 5^{15} r_n \pmod{2^{35}}$$

The period of each of the sequences is 2^{33} as shown by the theory of numbers[7]. Number sequences generated in this manner have been tested by Juncosa for statistical correlation with lags of 1 and 3, and for frequency of special bit groups[8]. Juncosa concluded that this is a satisfactory method for providing pseudo-random number sequences. Care is taken to avoid using bit groups near the low-order end of the numbers since short periods would be encountered there.

GEOMETRY

The geometry routine determines the position of a neutron each time there is a collision and whenever a regional boundary is crossed. After the path length is selected in a given region, tests are made to determine if a boundary is reached before the path length is spent. If so, the coordinates of the point of crossing are computed and the region number is adjusted to that of the new region. A new value of the path length is found so that the neutron path is resumed, with the same direction cosines as before, in the new region. The path length is found by the formula $-\frac{1}{\Sigma_t} \ln r$, where $\frac{1}{\Sigma_t}$ is the mean free path of the neutron in the region at the energy involved, and r is a random number in the range from 0 to 1.

The computation is effected in a rectangular cell that has a cylindrical fuel assembly at its center. A schematic view of the cell arrangement as observed in a horizontal plane is presented in Figure 2. The base of each rectangle is parallel to the x axis. A rectangular coordinate

system is used, with the z axis taken as the axial center of a fuel assembly. For each collision the position relative to the center of an individual cell is found, and the x,y coordinates of the center of the cell, initially (0,0), are adjusted upon entry into a new rectangle.

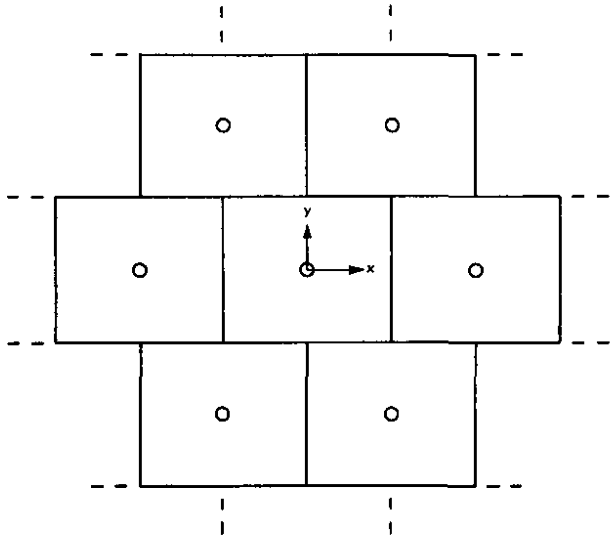


FIGURE 2 - GEOMETRIC ARRANGEMENT OF CELLS

Logic for the geometry routine appears in Flowsheets 3 and 4. The method of determining whether or not a boundary of a cylindrical region is reached before a collision is basically that of Cashwell and Everett.[9] By the method of comparing the squares of radii the procedure avoids taking the square root of a discriminant whenever a collision is accomplished; i.e., the distance to a boundary does not need to be calculated.

SCATTERING PROCEDURE

The scattering routine picks from tables the mean free path and ratios of cross sections that are used in determining the mass of the target atom and compiling absorption statistics. An index for the cross section tables is found by a method used by Coveyou and Carter.[10] The minimum value of the energy in a band, an even power of 2 in floating binary form, is subtracted from the floating binary value of the energy. Then seven of the eight leading binary bits of the remainder are retained as an index. This index is used to select the mean free path from tables, of 128 entries each, provided by the input tape. The program then refers to the geometry routine to determine if the probability-weighted mean free path is used up before a regional boundary is encountered. If so, a collision occurs and the calculation proceeds to one of five sections of the collision routine, depending on the pertinent isotopic mixture. Again the index is used in determination of the target atom and its effective mass.

The probability, p_i, of an event of type i occurring among j competing events is

$$p_i = \frac{\Sigma_i}{\sum_j \Sigma_j},$$

where Σ_i and the Σ_j are macroscopic cross sections in the laboratory frame of reference. The input tape provides tables of p_i for both scattering and absorption as a function of material and energy. An event is of type i if a number r, selected at random from the range 0 to 1, is in the interval

$$\sum_{j=1}^{i-1} p_j \leq r < \sum_{j=1}^{i} p_j$$

After the type of event is determined, the code assigns the value of the scattering mass. Only scattering events are selected by the above method since a weighting technique is employed which makes use of the survival probability, $S = \Sigma_s/\Sigma_t$, in tabulating absorption and terminating neutrons.

Effective Mass

Chemical binding of the target atoms in a water moderator increases the inertia of the target in collision. The influence of this effect is approximated in the calculation by using a larger mass for the target atom. When the incident neutron has energy in excess of the vibrational binding energy of the molecule, E*, it is assumed that the target is unbound and free atom masses are used. If the energy of the incident neutron is less than E*, the effective masses derived by Brown and St. John are employed.[15] Thus, in D_2O, the effective mass of oxygen, A(O), is 16 and that of deuterium, A(D), is 2 for events occurring above E* = 0.143 ev. A(O) is 20 and A(D) is 3.6 for events occurring below E*. Similarly for H_2O, A(O) is 18 and A(H) is 1.9 for events occurring below E* = 0.226 ev.

An evaluation of low energy scattering parameters for oxygen and deuterium in D_2O at energies ranging from 0.008 to 0.1 ev has been made by Spielberg.[11] Similar evaluations have been reported by Tralli, et al., for low energy scattering in H_2O.[12] Spielberg has reported, for example, that A(D) = 19.751 at 0.008 ev, 4.8910 at 0.025 ev, and 3.3887 at 0.06 ev. A(O) is given as 20.00 at energies of 0.025 ev and below, and 16.00 at 0.20 ev and above, with other values at discrete energies between these limits. The effect of these target masses on slowing down distributions could be studied by the Casino 13 code.

Weighting Procedure

If a neutron collides with a nucleus in an isotopic mixture having an absorption cross section, there is a probability p_a of capture. In a Monte Carlo program, absorption may be tabulated in either of two ways. (1) A random number r is selected in the range from 0 to 1 and the whole neutron is said to be absorbed if $0 \leq r < p_a$. (2) A weight parameter, W, initially 1, may be used, tallying $p_a W$ in the proper category at each collision and continuing with a neutron weight of $(1 - p_a)W$. The latter method is used by the Casino 13 code with the provision that when the weight of the incident neutron becomes less than an arbitrary value, say 0.5, "Russian roulette" is played. This is accomplished by picking a random number and testing to see if $r < W$. If not, the neutron is continued with W restored to 1; otherwise the neutron is assigned a weight of 0 and its history is terminated.

Target Velocity

The treatment of target velocities and collision mechanics in Casino 13 is similar to that used by Brown, and with the exception of the high energy mechanics the following discussion of these subjects is adopted from the reference given.[6] The procedure is shown in Flowsheet 5.

The probability, p, of collision between a neutron of velocity $\vec{u}$ and a target of velocity $\vec{U}$ depends upon the relative velocity and the thermal distribution of the target atom velocities. It is customary to assume that the target atoms possess a Maxwellian distribution of velocities, $M(\vec{U})$, in the laboratory system and that the scattering cross section in the center-of-mass coordinates is independent of the target velocity. The probability of collision with a moderator atom is obtained by integrating over all possible velocities

$$p\, d\vec{U} = \int_0^\infty |\vec{u} - \vec{U}| M(\vec{U})\, d\vec{U}$$

$$= \frac{1}{\beta \sqrt{\pi}} e^{-\beta^2 u^2} + \left(\frac{1}{2\beta^2 u} + u\right) \mathrm{Erf}(\beta u)$$

where $\beta^2 = \frac{A}{2kT}$, kT represents the moderator temperature, and $\mathrm{Erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy$ is the error function. The target velocity must be selected from equally weighted samples of this integral probability.

Since the integral probability is complex and difficult to decompose into equally weighted samples, the differential probability is dealt

with instead. The selection of U is performed by a rejection technique. An upper bound of the integrand is u + U. Thus, an upper bound of the probability is

$$\int p_{max}\, d\vec{U} = u \int_0^\infty M(U)dU + \int_0^\infty U\, M(U)dU$$

$$= u(1) + \frac{2}{\sqrt{\pi}}\sqrt{\frac{kT}{A}}$$

$$\equiv u + I$$

A random number r_1 is drawn to decide the selection of U. If $r_1 \leq \frac{u}{u + I}$, a value of U is taken at random from a table biased with a Maxwellian distribution. If $r_1 > \frac{u}{u + I}$, U is selected from a table biased with a U-weighted Maxwellian distribution. Although the U so obtained is representative of the upper bound probability, p_{max}, the actual probability is more restrictive. Every speed U is chosen too frequently by the p_{max} sampling. The frequency should be reduced by the fraction by which p_{max} exceeds the actual p. Thus a second random number, r_2, is drawn to test the choice of U. If $r_2 \leq \frac{|\vec{u} - \vec{U}|}{u + U}$, U is accepted as the target speed. Otherwise the sample is rejected and another is chosen in the same manner.

COLLISION MECHANICS

The equations of neutron scattering are taken from a simple model using classical mechanics. Details of the j^{th} neutron collision with the moderator atoms are derived from the conservation of energy and momentum. Upon collision, the following scattering data are calculated sequentially to obtain the energy loss and the scattering angle.

$$x_j^2 = \frac{1}{(A_j + 1)^2}\left[u_j^2 + A_j^2U_j^2 + 2A_ju_jU_j \cos a_j\right]$$

$$v_j^2 = \frac{A_j^2}{(A_j + 1)^2}\left[u_j^2 + U_j^2 - 2u_jU_j \cos a_j\right]$$

$$E_{j+1} = x_j^2 + v_j^2 + 2x_jv_j \cos b_j$$

$$\cos c_j = \frac{1}{x_j(A_j + 1)}\left[u_j + A_jU_j \cos a_j\right]$$

$$\cos \psi_j = \cos b_j \cos c_j + \sin b_j \sin c_j \cos \Phi_j$$

$$\mu_j = \frac{1}{u_{j+1}} \left[v_j \cos \psi_j + x_j \cos c_j \right]$$

The flight parameters are defined as follows:

$\vec{x}$ - velocity of the center of mass of the collision system

$\vec{v}$ - velocity of the neutron in the barycentric system after collision

A - effective mass of the target

a - angle between $\vec{u}$ and $\vec{U}$

b - angle between $\vec{x}$ and $\vec{v}$

c - angle between $\vec{x}$ and $\vec{u}$

ψ - angle between $\vec{v}$ and $\vec{u}$

μ - cosine of the angle between $\vec{u}_j$ and $\vec{u}_{j+1}$

Φ - azimuth of $\vec{v}$ around $\vec{x}$

E_j - energy of the neutron entering the j^{th} collision

The mass of the neutron is taken as unity and the units of velocity are such that $u = \sqrt{E}$. The index j is the number of the collision. The solid angle of scattering in the barycentric system (i.e., Φ and cos b) is selected at random.

At energies much greater than thermal, it is not useful to consider the velocity of the target nucleus. If U = 0 in the above formulas, the following simplified equations of high energy scattering are obtained.

$$E_{j+1} = \frac{A^2 + 2A \cos b + 1}{(A + 1)^2} E_j$$

$$\mu_j = \frac{A \cos b + 1}{(A^2 + 2A \cos b + 1)^{\frac{1}{2}}}$$

These formulas are used by Casino 13 at energies above an arbitrary value as determined by an input parameter.

DIRECTION COSINES

The direction cosine subroutine obtains the parameters $(\lambda_1, \mu_1, \nu_1)$ of a neutron after each collision. It is assumed that the neutron is scattered through a laboratory angle ω from an incident direction (λ, μ, ν). The amount of rotation about the incident vector is determined by the azimuthal angle Φ, which is picked at random such that $0 \leq \Phi < 2\pi$. The initial value of the cosine of ω for each neutron is selected randomly by the source routine from the distribution

$(2r - 1)$, where r is a random number on the interval $0 \leq r < 1$. Succeeding values of cos ω are developed by the collision mechanics routines.

In order to obtain the values of $(\lambda_1, \mu_1, \nu_1)$, the direction cosines (u, v, w) are obtained relative to the initial vector, which is taken for convenience to lie on the positive y axis of a Cartesian coordinate system. The direction cosines (λ, μ, ν) of the incident vector, relative to fixed x,y,z axes, are used together with u, v, and w in a composite rotation matrix to form λ_1, μ_1, and ν_1.

The formulas for u, v, and w are

$$u = \sin \omega \cos \phi$$

$$v = \cos \omega$$

$$w = \sin \omega \sin \phi$$

The rotation is accomplished by the formulas

$$\lambda_1 = \frac{\mu}{\rho} u + \lambda v - \frac{\lambda \nu}{\rho} w$$

$$\mu_1 = \frac{-\lambda}{\rho} u + \mu v - \frac{\mu \nu}{\rho} w$$

$$\nu_1 = 0 + \nu v + \rho w$$

where

$$\rho = \sqrt{1 - \nu^2}$$

A special procedure is used so that if ρ^2 is very small (for example, $\rho^2 < 0.001$), the rotation is about the z axis and there is no rotation of axes. This prevents dividing by an effective zero and taking the square root of a very small number. In this abbreviated routine the formulas become

$$\lambda_1 = \sin \omega \cos \phi$$

$$\mu_1 = \sin \omega \sin \phi$$

$$\nu_1 = \nu \cos \omega$$

ANALYSIS

The collision data generated in the course of neutron histories are analyzed to obtain the number of absorptions in each region, the neutron age and migration area, and the flux as a function of position energy and direction. The analysis coding is based on a uniform hexagonal lattice, and would have to be revised if any other lattice pattern were considered. The number of fissions and absorptions in each of the components of the fuel assembly and in the surrounding

moderator are tabulated according to energy into thermal absorptions (below 0.56 ev) and fast absorptions (above 0.56 ev). From these quantities, values of the thermal utilization, f, and the multiplication constant, k_∞, can be calculated.

The orthogonal components of the neutron age and migration area are computed using the following equations:

$$\tau(E_k)_x = \sum_i \frac{W_i (x_i - x_o)^2}{6 \sum_i W_i}$$

$$M_x^2 = \frac{\sum W_{abs,j} (x_j - x_o)^2}{6 \sum_j W_{abs,j}}$$

where W_i is the weight of the i^{th} neutron when its energy drops below E_k, $W_{abs,j}$ is the weight of the neutron absorbed in the j^{th} collision, and x_o is the x coordinate of the neutron at birth.

Values of τ and M^2 in the y and z directions are calculated in the same manner. The neutron age, τ_k, is calculated for four values of the energy, E_k.

The flux is tabulated for 18 energy groups and for a maximum of 32 spatial regions including a maximum of 12 within the fuel assembly. The moderator outside the fuel assembly is divided radially into 5 regions and azimuthally into 4 sections, giving a total of 20 regions. In each group the flux is given by the equation

$$\Phi(E,r) = \frac{1}{(V)\Delta E} \sum_j \frac{W_j}{\Sigma_j}$$

where W_j is the neutron weight, Σ_j is the total macroscopic cross section of the isotopic mixture containing the target nucleus at the j^{th} collision, V is a number proportional to the volume of the region, and ΔE is the width of the energy group.

The procedure for tabulating the neutron flux is depicted by Flowsheets 6 and 7. Figure 3 is used in developing the scheme for "hexagonalizing" the rectangular cell, and Figure 4 displays typical radial and azimuthal regions for which flux is tabulated. At each collision the flux is added to a cumulative sum corresponding to one of 6 directional categories, one of 32 regions, and one of 18 energy groups. The flux is added to a similar sum to get the total flux for each energy group and region. Flux summations are carried throughout the calculation and printed in the final edit at the end of a run.

In Figure 4 the region numbers run from 1 to 31. Another region may be obtained by dividing an arbitrary cylindrical region radially in the tabulation. The data corresponding to the inner section of the divided region will be tabulated in a category with index 0 to complete the total of 32 regions.

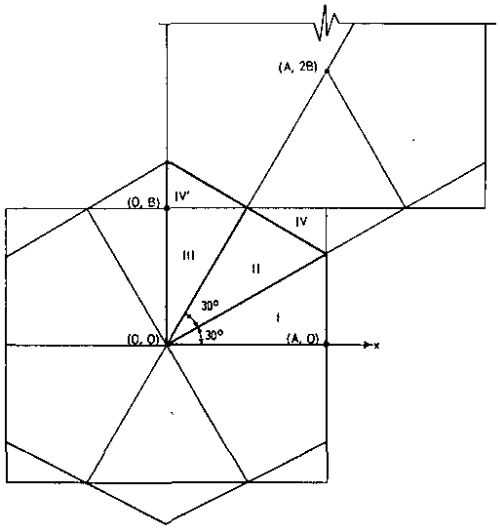


FIGURE 3 - HEXAGONALIZED CELL

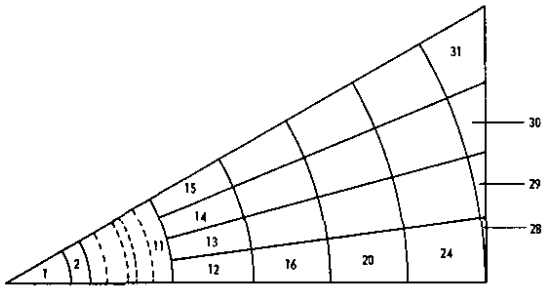


FIGURE 4 - FLUX REGIONS

In Figure 3 one sees that triangle IV belongs to the rectangular cell with center at (0,0) and to the hexagonal cell with center at (A,2B). Triangle IV is therefore rotated 180° until it coincides with triangle IV', where it becomes part of hexagon (0,0) and triangle III. The signs of the x and y coordinates are then changed since they have an opposite sense with respect to the new center. Because of cylindrical symmetry in the fuel components, tabulation is restricted to the first quadrant and then compressed into the first 30°, represented by triangle I, Figure 3.

As seen from Figure 4, the region for tabulation is a function of radius and azimuthal angle. The radius, r', is taken as $(x'^2 + y'^2)^{\frac{1}{2}}$ and the angle of rotation is given by $\sin\theta = y'/r'$ and $\cos\theta = x'/r'$, where x' and y' are the x and y components of the radius vector after possible transformation involving triangle IV, Figure 3. The direction cosines λ' and μ' relative to the radius vector are found by a rotation of axes through the angle θ about the z axis. The azimuthal angle is restricted to the first quadrant by the use of magnitudes of $\sin\theta$ and $\cos\theta$, and if the point (r',θ') falls in triangle III, θ is reduced by 60°. If (r',θ') lies in triangle II, the $\sin\theta$ and $\cos\theta$ are interchanged and θ' is reduced by 30°.

The direction of the flux relative to the radius vector is determined by (λ', μ', ν). Some work is avoided by adding all the flux at the collision to a sum in one of 6 directional categories rather than assigning parts proportional to λ', μ', and ν to separate categories. The magnitude and sign of the largest direction cosine determine the category.

EDITING AND RECYCLING

After a neutron has undergone a collision and its new energy and direction are determined, considerable bookkeeping is needed in preserving collision data and in preparation for the succeeding collision. The steps which are taken are shown in Flowsheet 2. For every collision the weight, spatial coordinates, and energy are placed in permanent history storages. The neutron may have been terminated or scattered into an energy outside the band in which neutrons are being processed. If neither of these things has occurred the neutron re-enters the collision process.

If the neutron history has been terminated, its weight is 0 and another neutron will be selected. The new neutron will be initiated by the source routine if the calculation is in band 1, or be resumed by means of the data in permanent history storages when calculation is in band 2 or band 3. In the latter case the energy and weight of the selected neutron are tested to assure that a history is not continued unnecessarily. In the former case the point of return to the source routine is dependent on whether or not 12 neutrons have already been started with the current fission energy. Whenever the neutron is scattered into an energy outside the band under consideration, the direction cosines are sent to the permanent history storages.

The index accumulator, IA1, used for reference to the history storages is adjusted by nine each time a new neutron is acquired, because the permanent data requires nine storages per neutron. When the contents of IA1 becomes ≤ 9, 300 neutrons have been carried through an energy band. Another record from the cross section tape is read, IA1 is restored to 2700, and the energy band number is increased by 1. If band 3 has just been completed, the input tape is rewound before the above steps and control is returned to the source routine for initiating the next 300. But the end of a batch may have been reached, in which case a summary of the absorption data, migration area, and neutron age for 600 neutrons is printed. A memory dump and record of machine status are obtained on a binary tape by means of the NU SOS subroutine after each completion of energy band 3.[14] This is useful for restart in case of machine malfunction or an unexpected interruption of the computation. The end of the computation is realized by testing Sense Light 1, which is turned on in the source routine after the last neutron of the last batch has been initiated.

When Sense Light 1 is found to be turned on after band 3 is finished, the program proceeds to the printing of the flux summaries. This consists of the total flux in each energy group, the entire contents of the flux tabulation storages, the moderator fluxes averaged over four azimuthal regions, and the total flux in each spatial region. The flux is summed over all spatial regions to obtain the total in each energy group, and over all energy groups for the total flux in each spatial region.

CROSS SECTION TAPE GENERATOR

A preliminary routine is used for preparing an input tape which is required by the Monte Carlo program, Casino 13. The cross section code is written in two parts, the expansion and the mix routines, which are discussed briefly below. Running time for this program is about 5 minutes.

EXPANSION ROUTINE

From a set of input tables of arbitrary length, the expansion routine produces tables of 128 values each. The expansion is made using the logarithmic interpolation formula,

$$\sigma_i = \sigma_0 \exp\left\{ \frac{\ln \frac{\sigma_1}{\sigma_0}}{\ln \frac{E_1}{E_0}} \ln \frac{E_i}{E_0} \right\}$$

In the above formula, E_i is a value of E between E_0 and E_1, and σ_i is a microscopic cross section corresponding to E_i, on the interval from σ_0 to σ_1. The formula is also used to extrapolate beyond the energy limits of the input table if the energy bounds of the expanded table are not contained in the input table.

Tables are expanded in each of three energy bands, the range of which is as follows:

Band 1: $2^8 \leq E \leq 1.875 \times 2^{23}$ ev

Band 2: $1 \leq E \leq 248$ ev

Band 3: $2^{-15} \leq E \leq 1.875$ ev

The input tables are made up of pairs of elements, the first of which is a cross section in barns and the second is the corresponding energy in ev units. Up to 15 such tables may be used for a given problem. Input values are taken from BNL-325, with the entries being read from the peaks and dips of the recorded plots and at suitable intermediate points.[13]

MIX ROUTINE

The mix routine computes macroscopic cross sections and combines them for the various elements in a mixture to obtain the total cross section, the mean free path, and the ratios of the individual cross sections to the total. Each of the values in the expanded tables is multiplied by a scaled concentration factor to obtain a macroscopic cross section. The above functions are then developed and arranged into tables in the order that is required by Casino 13. Upon completion, the tables are transcribed in binary form onto the input tape.

The tape is made up of three records - one for each energy band - of 2690 words each. The last two words of each record are values of energy. The first of these is used for determining an index for reference to the above tables within the scattering routine and the second is for cutoff at the lower energy limit of the band.

This is a special-purpose routine, written for a particular set of isotopic mixtures that are to be used in a reactor. The mix code is written for five mixtures, involving twelve tables of input data for energy band 3, and nine tables for each of bands 1 and 2.

INSTRUCTIONS FOR USING THE CASINO 13 CODE

The input data for Casino 13 are punched in SAP form, which is discussed in the Appendix.[17] The parameters pertinent to a specific subroutine are read in upon the first entry of the program into the subroutine. The quantities listed below are in the order in which they enter the machine.

1. The source routine requires 3 cards. The first of these contains:

SREG Number of the source region
NR 1 + the number of cylindrical regions
BTEST 1 + the number of batches in the run
x,y,z Spatial coordinates of the point source

The second source card contains a name generator, and the third contains a table of indices, RMAT. The numbers contained in RMAT correspond to the isotopic mixtures assigned to successive regions, starting with the moderator and proceeding inward toward the center of the cell. A typical set of source cards contains

```
DEC  7, 10, 2, 3.5, 0, 0
OCT  10001000
DEC  1, 2, 1, 3, 1, 3, 1, 2, 1
```

2. Input for the scattering routines consists of 30 values as defined below.

ESTAR	Energy below which D atom has increased mass
2STAR	Energy below which H atom has increased mass
ETAB	Energy below which tabulation is desired
ETH	Energy below which thermal absorptions occur
EIN	Energy below which target motion is applied
MASSI	6 values of isotopic masses
IAS	9 values of 2 $(kT/\pi A)^{\frac{1}{2}}$
UTS	9 values of $(kT/A)^{\frac{1}{2}}$
WCO	Neutron weight below which Russian roulette is played.

A sample of the above data is listed for 6 cards:

DEC	0.143, 0.226, 1.4E23, 0.56, 1.0
DEC	3.6, 20.0, 1.9, 235.0, 27.0, 12.0
DEC	0.1279106, 0.09533893, to 9 values on 2 cards
DEC	0.1133578, 0.08449193, to 9 values on 2 cards, and 0.5 as the last number on the sixth card.

3. Four values of cell dimensions are read in by the geometry routine followed by RTAB, the table of squared radii of the cylindrical regions. The dimensions are in the order A, 2B, 2A, B, and the values of r_i^2 are in the order 0, r_1^2, r_2^2, ----, r_n^2 where n is the total number of cylindrical regions. Both the dimensions and r_1^2 are to be punched in floating decimal form.

4. A total of 24 input values are needed for tabulation purposes. These include 17 words of energy in ascending order to define the energy groups, and 2 words to define a cylindrical region, which will be divided at the radius whose square follows the region number. The next 2 numbers are the slope and y intercept of the line, as shown in Figure 3, above which all points in triangle IV lie. The final 3 words are squares of the radii in the moderator which define the regions of tabulation outside the fuel as shown in Figure 4. All the above data, with the exception of the divided region number, are to be punched in floating decimal form.

MACHINE PROCEDURE

Load the cross section tape on the tape unit 4. Load a tape for the SOS dump on tape unit 5. Set Sense Switches 2 and 3 to the DOWN position. Clear memory and then load cards.

The order of the deck is BOL, binary program deck, and the data cards in the order described above, where BOL is a loading program for binary or octal cards.[19]

If it is desired to change any of the binary instructions or a fixed constant in the program deck, correction cards may be inserted before the transfer card. A correction card is made up with the octal address in columns 1-5 and the octal form of the correction in columns 37-48, with column 37 double-punched in case of a negative sign.

Printing of collision data may be obtained, one line per collision, by depressing Sense Switch 4. The seven words in the printed line are energy, x, y, z, weight, mean free path, and "won". The value of won is 0 unless Russian roulette was played on the collision and won, in which case its value is 1.

A restart after program interruption is effected by mounting the SOS tape on tape unit 1, setting the sense switches to their usual positions, clearing memory, and then depressing the Load Tape button.

USE OF CROSS SECTION TAPE GENERATOR

Input data cards are to be placed behind the binary program deck in the following order:

1. N3 to N8
2. TAB1, TAB2, TAB3
3. TL1, TL2, TL3
4. Concentrations

Each of these data categories is explained below.

1. N3, N4, and N5 are the number of tables of input for the 3rd, 2nd, and 1st energy bands, respectively. The total number of values per energy band in the above tables is N6, N7, and N8.

2. TAB1 is a set of tables made up of pairs of values, σ_i and E_i, starting from very low energy and proceeding (in ascending order) to E in the range of 1.875 ev. The values σ_i are the microscopic cross sections corresponding to E_i. The tables are of arbitrary length, not exceeding 256. TAB2 extends from E = 1 ev to E = 248 ev, and TAB3 extends from E = 256 ev to E = 15.7 Mev. The latter are of the same form as TAB1.

3. TL1 is a list of N3 entries, which are the number of input values for each of the respective tables in TAB1. TL2 and TL3 are related to TAB2 and TAB3 in like manner.

4. The number of nuclei per unit volume of the isotopes is scaled by a factor of 10^{-24} to compensate for the fact that the input cross sections are in units of barns. Ten entries correspond to the elements contained in five isotopic mixtures.

MACHINE PROCEDURE FOR TAPE GENERATOR

Load a blank tape on tape unit 4 to contain the output.

Set Sense Switch 2 to the DOWN position.

Clear memory and then load cards.

The order of the deck is ABL, binary program deck, and data cards, where ABL is a loading program for binary cards.[14]

W. V. Baxter

W. V. Baxter
Theoretical Physics Division

BIBLIOGRAPHY

1. Ehrlich, R. and Hurwitz, H., Jr., "Multigroup Methods for Neutron Diffusion Problems". Nucleonics 12, No. 2, 23-30 (1954).

2. Weinberg, A. M. and Wigner, E. P., The Physical Theory of Neutron Chain Reactors. Chicago, Ill.: The University of Chicago Press (1958) pp. 219-78.

3. Cashwell, E. D., Everett, C. J., and Rechard, O. W., A Practical Manual on the Monte Carlo Method for Random Walk Problems. Los Alamos Scientific Lab., LA-2120, January 1957.

4. Van Norton, R., A Preliminary Description of an NYU Resonance Escape Probability Monte Carlo Program (704). 4 Wash. Pl., New York 3, N. Y., AEC Computing and Mathematics Center, Stencil No. S-570905.

5. Beeler, J. R. and Ryan, J. W., Monte Carlo Research Series: Basic Three-Dimensional Monte Carlo Program for Cylindrical Geometry, Part I: Physics and Method. General Electric, APEX-374, January 1958.

6. Brown, H. D., "A Monte Carlo Study of Neutron Thermalization". J. Nuclear Energy 8, 177-86 (1959).

7. Jones, B. W., The Theory of Numbers. New York: Rinehart (1955) p. 116.

8. Juncosa, M. L., Random Number Generation on the BRL High-Speed Computing Machines. Ballistic Research Lab., BRL-855, May 1953.

9. Cashwell, E. D. and Everett, C. J., op. cit., 74-78.

10. Coveyou, R. R. and Carter, H. P., personal communication.

11. Spielberg, D., "Neutron Cross Sections of Deuterium and D_2O for Multigroup Calculations". A Supplement to Nuclear Sci. and Eng., 1, No. 2, December 1958, pp. 155-6.

12. Tralli, N., Some Neutron Cross Sections for Multigroup Calculations. General Electric, APEX-467, June 30, 1958.

13. Hughes, D. J. and Schwartz, R. B., Neutron Cross Sections. Brookhaven National Lab., BNL-325, 2nd. Ed., July 1, 1958.

14. ABL: Absolute Binary Loader. 4 Wash. Pl., New York 3, N. Y., AEC Computing and Mathematics Center, Stencil No. 0-570517.

15. Brown, H. D. and St. John, D. S., Neutron Energy Spectrum in D_2O. E. I. du Pont de Nemours & Co., DP-33, February 1954.

16. NU SOS: Save and Restore Routine. 4 Wash. Pl., New York 3, N. Y., AEC Computing and Mathematics Center, Stencil No. 0-580702.

17. Mealy, G. H., 704 Symbolic Assembly Program - UA SAP 3-7. 4 Wash. Pl., New York 3, N. Y., AEC Computing and Mathematics Center, Stencil No. 0-590120.

18. Goldberg, B., NU INP1: Generalized Input Program. 4 Wash. Pl., New York 3, N. Y., AEC Computing and Mathematics Center, Stencil No. 0-570826.

19. BOL: Binary and Octal Card Loader. 4 Wash. Pl., New York 3, N. Y., AEC Computing and Mathematics Center, Stencil No. 0-570720.

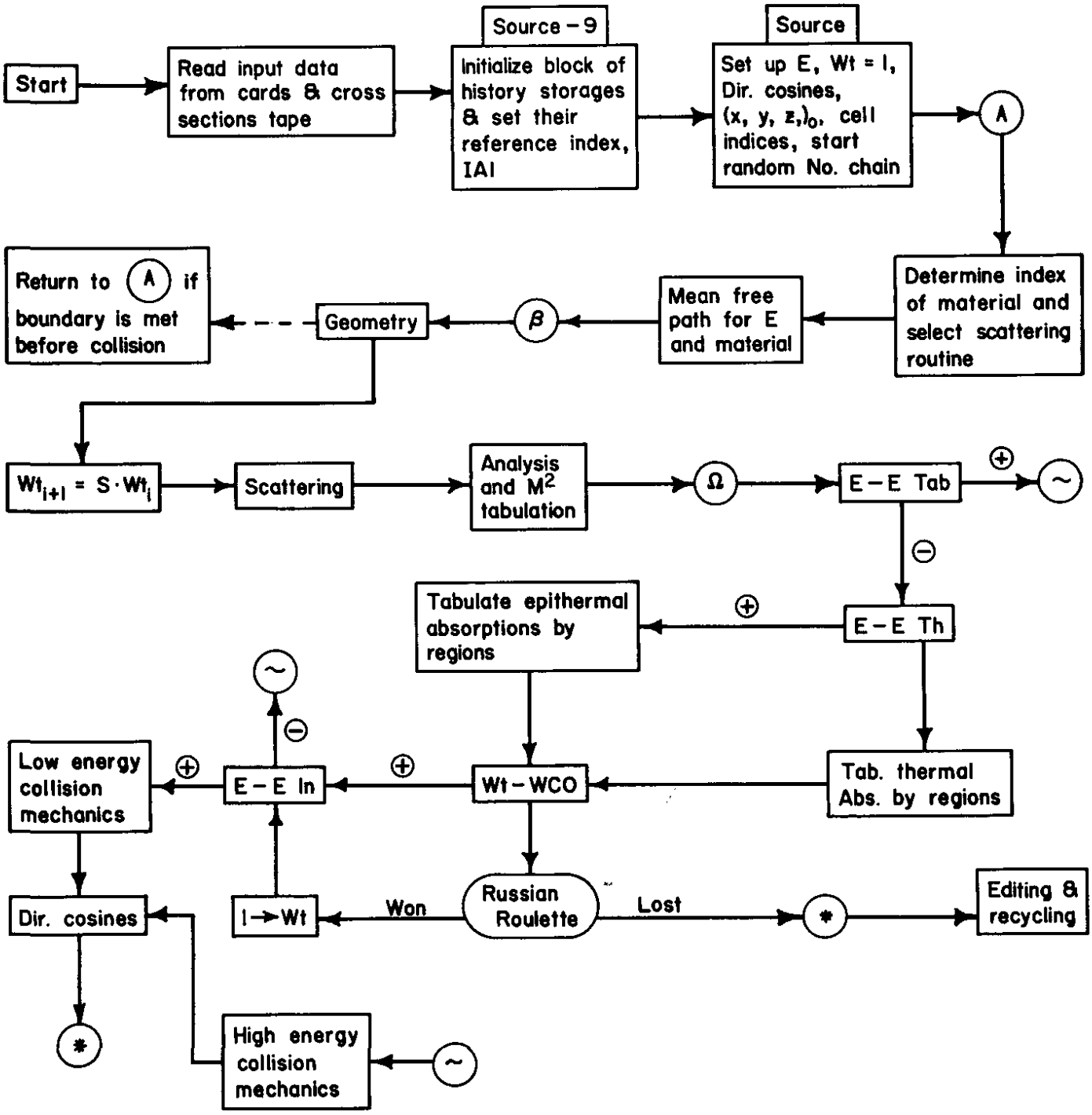
NOMENCLATURE

English Letter

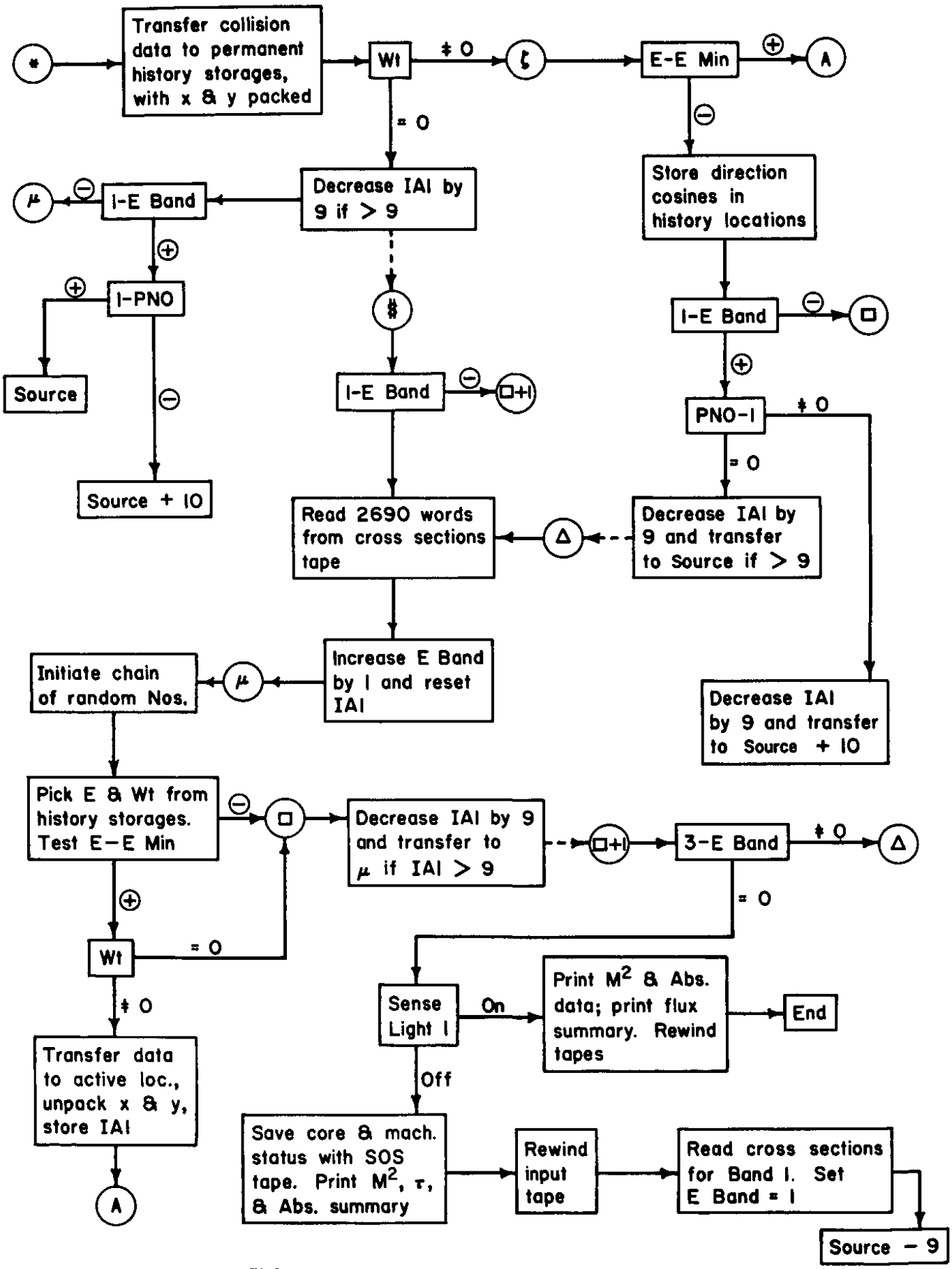
A	effective atomic mass of the target atom
A(O)	effective atomic mass of the oxygen atom
A(D)	effective atomic mass of the deuterium atom
(A,B)	half-dimensions of the rectangular cell used in the lattice
E*	energy below which the atoms in D_2O have an increased effective mass.
E**	similar energy for atoms in H_2O
E_j	energy of a neutron entering the j^{th} collision
E_k	energy at which the Fermi age is computed
kT	moderator temperature
k_∞	infinite multiplication factor of a lattice
M^2	migration area
(M_1,M_2)	x,y coordinates of the center of the cell in which calculation is being effected
p_i	probability of an event of type i
r	a random number on the range $0 < r < 1$
r'	in tabulation, the magnitude of the projected radius vector
S	survival probability, $= \Sigma_s/\Sigma_t$
$\vec{u}$	velocity of the incident neutron
$\vec{U}$	velocity of the target atom
$\vec{x}$	velocity of the center of mass of the collision system
$\vec{v}$	velocity of the neutron in the center of mass system after collision
V	a number proportional to the volume of a region used in flux tabulation
W, or Wt	neutron weight, initially 1

Greek Letter

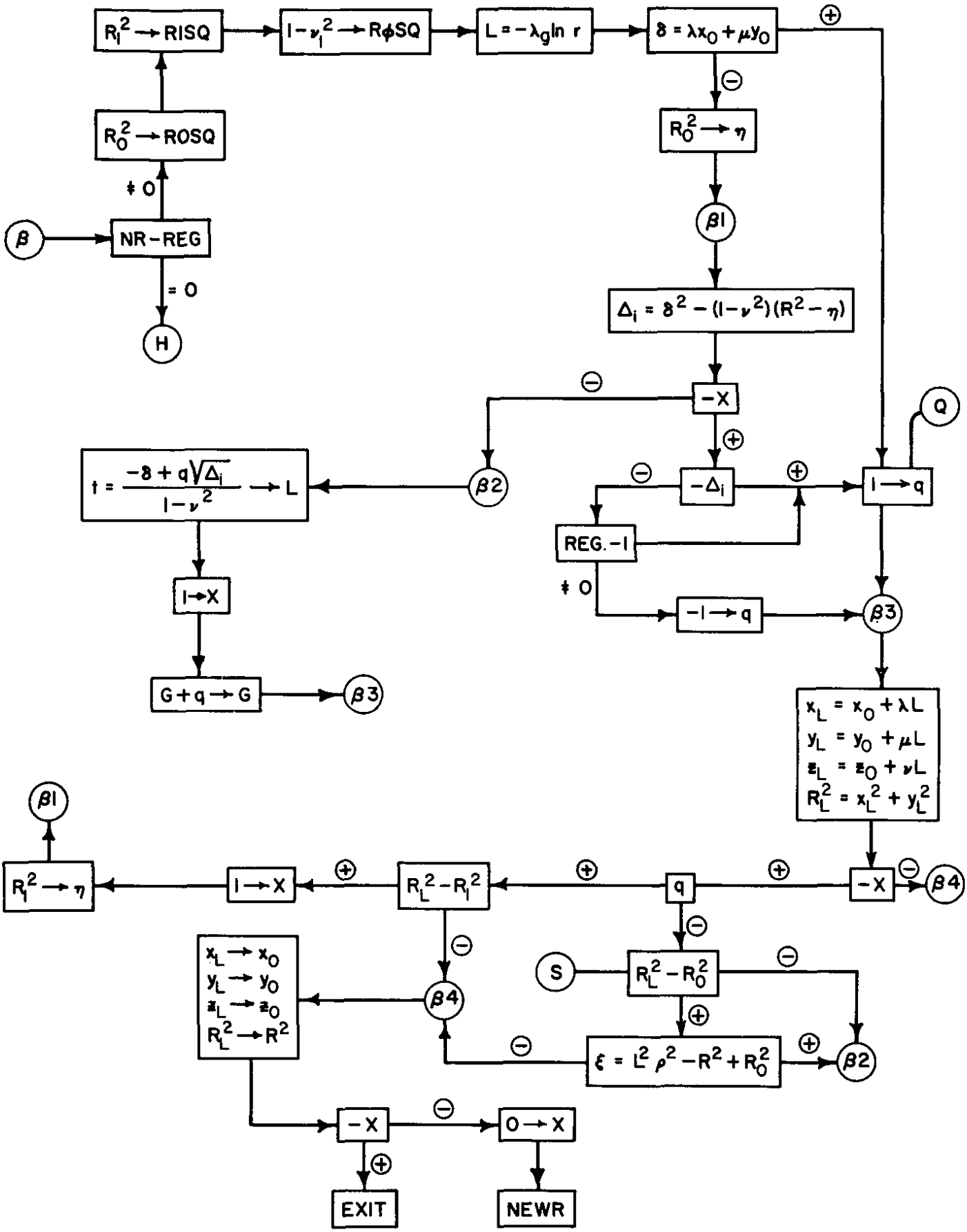
θ	any polar angle - in tabulation, the angle between the positive x axis and the projected radius vector
ϕ	an azimuthal angle or angle of rotation - azimuth of $\vec{v}$ around $\vec{x}$
(λ,μ,ν)	general direction cosines
(λ',μ')	direction cosines relative to the radius vector after rotation of axes through the angle θ around the z axis
θ'	first quardrant angle resulting when absolute values of sin θ and cos θ are used in the flux tabulation
ρ	$(1 - \nu^2)^{\frac{1}{2}}$, where ν is the third direction cosine
τ	Fermi age
σ	a microscopic cross section
Σ	a macroscopic cross section
Σ_t	reciprocal of the mean free path
ω	laboratory scattering angle
μ	cosine of ω
ψ	angle between $\vec{v}$ and $\vec{u}$



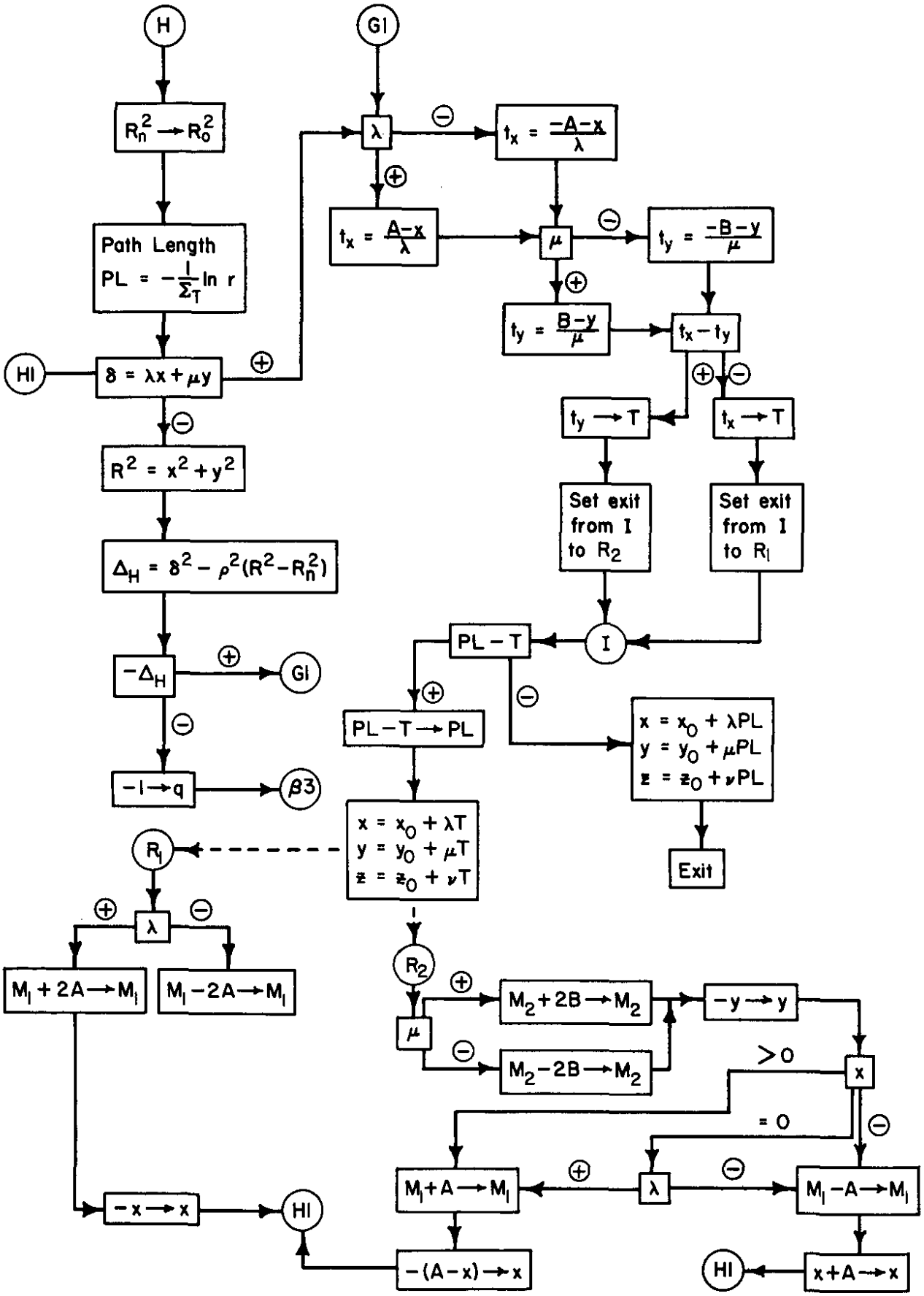
FLOWSHEET 1 – CASINO 13 PROCEDURE



FLOWSHEET 2 - EDITING AND RECYCLING

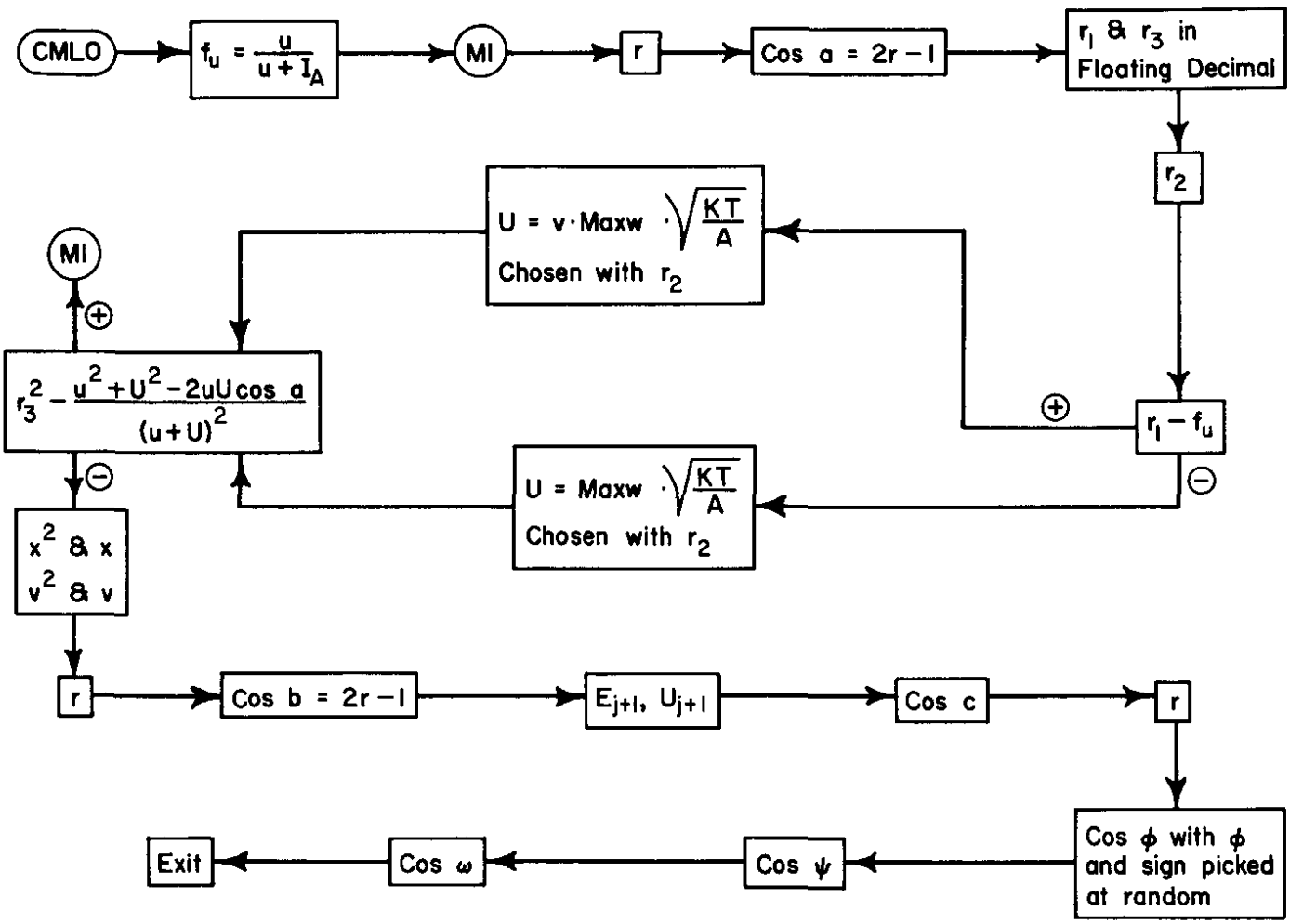


FLOWSHEET 3 - CYLINDRICAL GEOMETRY

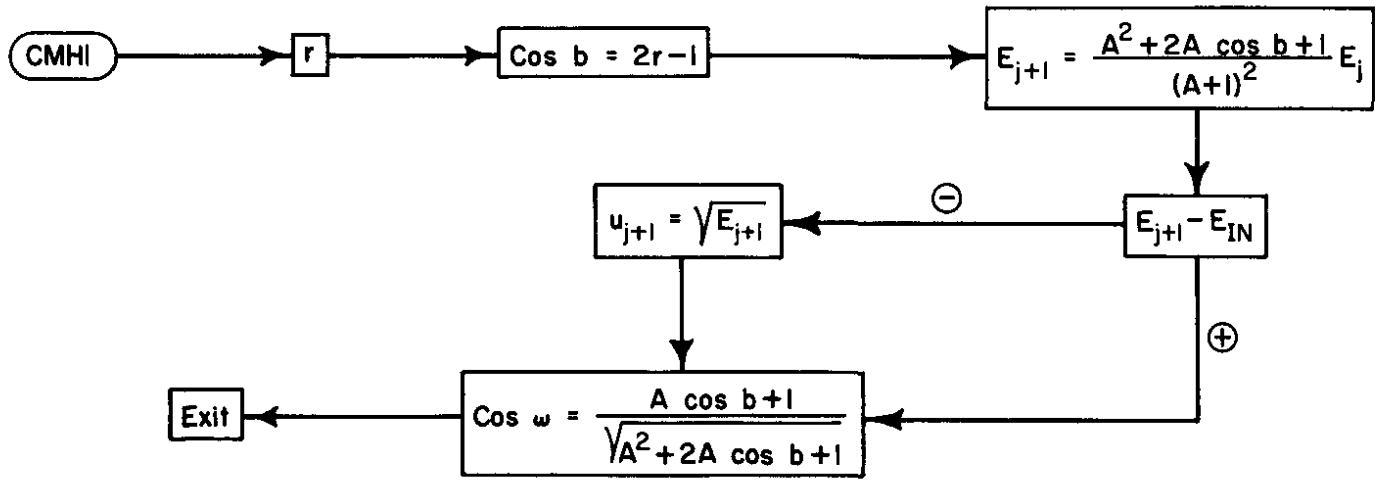


FLOWSHEET 4 – RECTANGULAR GEOMETRY

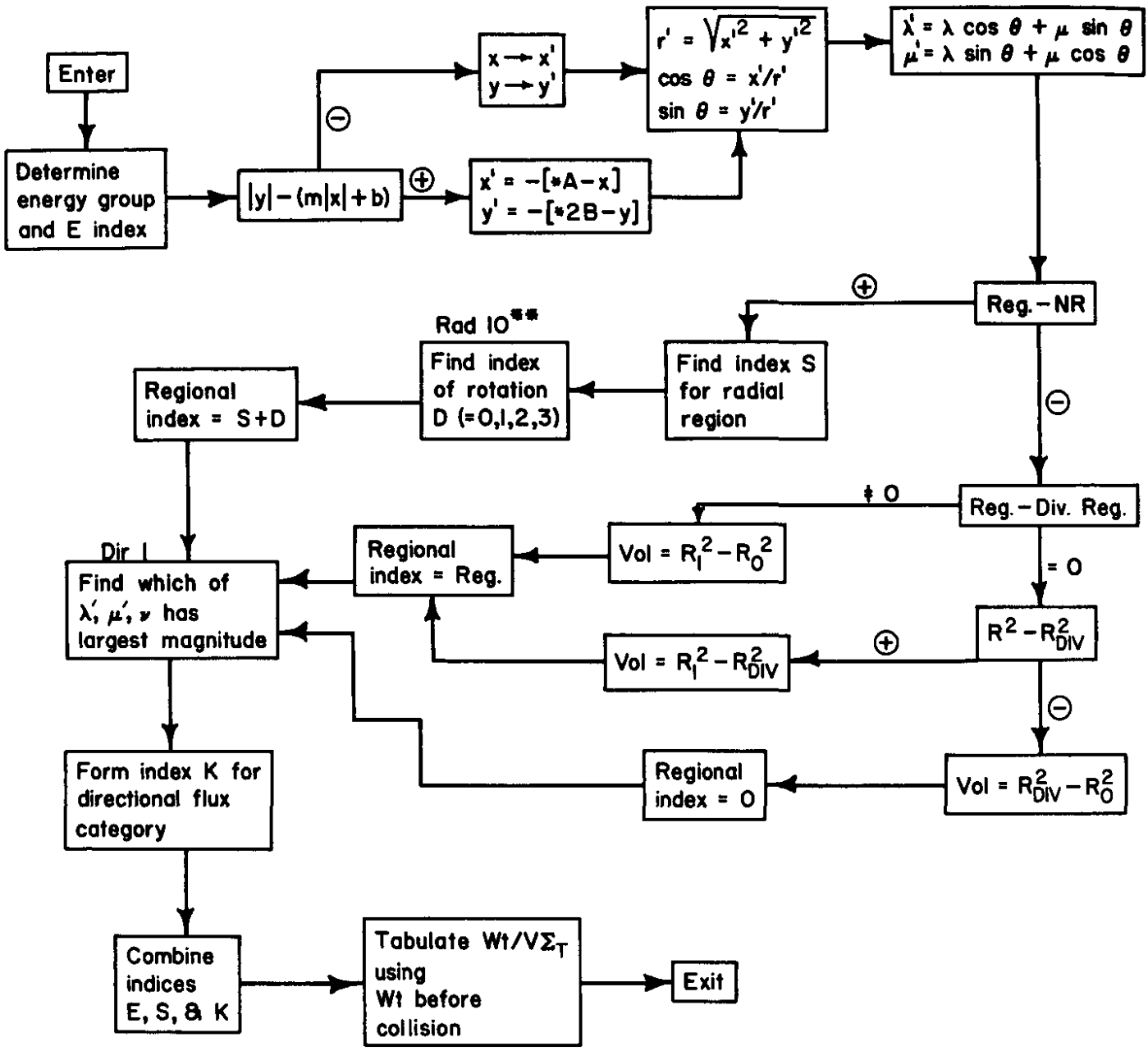
Low Energy



High Energy



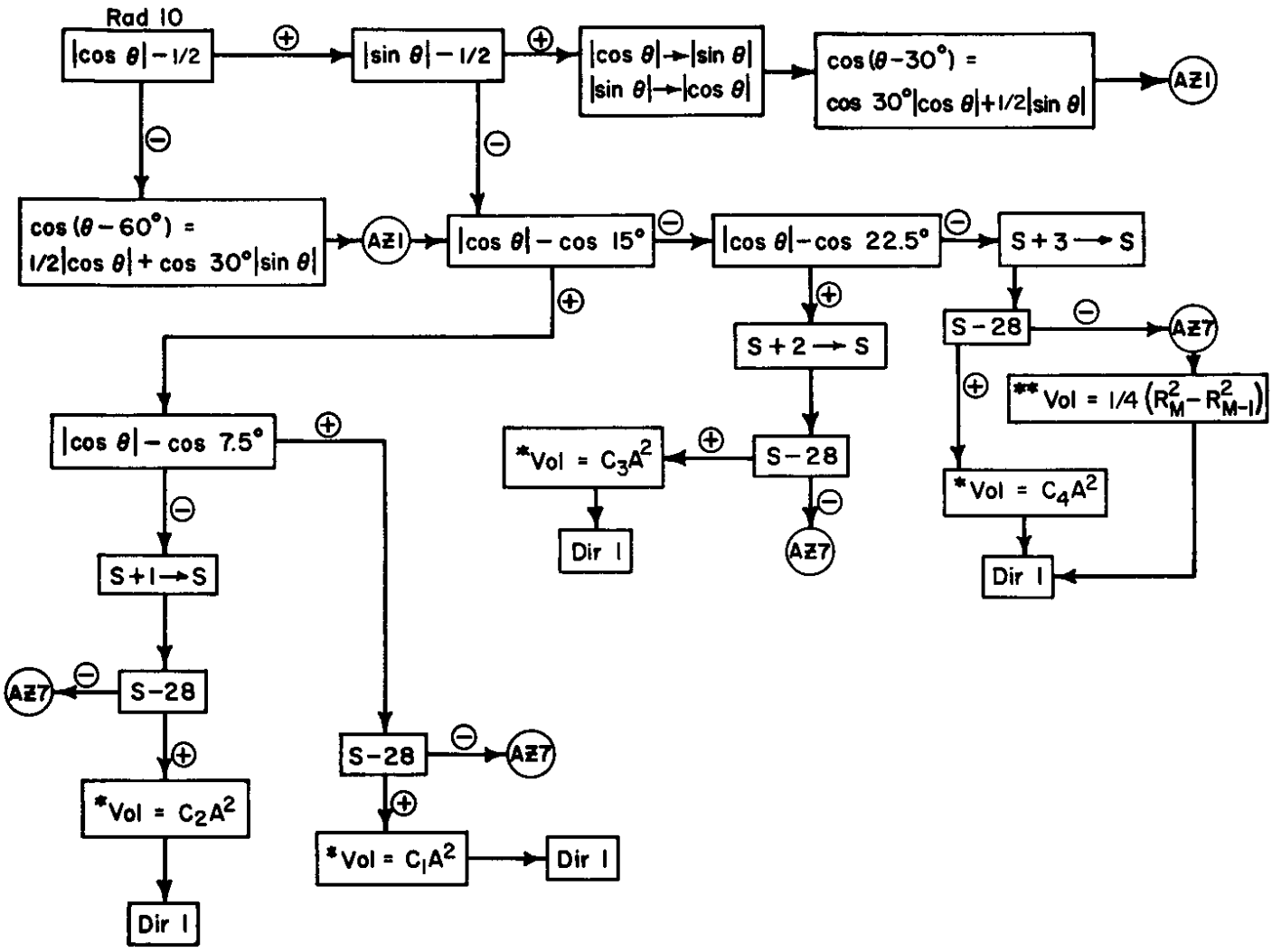
FLOWSHEET 5 – COLLISION MECHANICS



*A is A prefixed by the sign of x, and
*2B is 2B prefixed by the sign of y.

**Refer to next flowsheet.

FLOWSHEET 6 – TABULATION OF ΔE_i · FLUX



*C_1, C_2, C_3, and C_4 are Volume Factors for Regions 28-31.

**R_M is a radius in the moderator.

FLOWSHEET 7 - AZIMUTHAL FLUX REGIONS

APPENDIX

FORMAT FOR INPUT CARDS

The input cards for Casino 13 are made up in the conventional SAP form.[17] Columns 1-6 are left blank since the calling sequence for INP1 assigns the location of the data which is being read.[18] DEC appears in columns 8-10 and data are in columns 12-72.

Successive words of data on a card are separated by commas, and the first blank to the right of column 12 indicates that all punching to the right of this blank is a remark. No word will be entered as data if it is interpreted as a remark. The last word of data on a card should not be followed by a comma.

If either a decimal point or the symbol E or both appear in a word of decimal data, the word is converted into a 704-type binary floating quantity. The decimal exponent used in this conversion is the signed number that follows immediately after the character E. If E does not appear, the exponent is determined by the location of the decimal point alone. For example, 3.2 E-3, 3.2×10^{-3}, and 0.0032 represent the same quantity, and 32E3, 3.2×10^{4}, and 32000.0 indicate the same number.

The absence of both E and the decimal point assures that the word will be entered as a binary fixed point quantity after conversion from fixed decimal form. Both fixed and floating decimal values may appear on the same card in any order. Words may be entered without conversion when they are in octal form by use of the pseudo-operation OCT in columns 8-10.