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Summary Report

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CAVEAT: A REVISED VERSION OF THE
GENERAL PURPOSE MONTE CARLO
PROGRAM, COHORT

Volume I - Theory and Techniques

by N. R. Byrn

October 1969
(Revised April 1970)

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CAVEAT: A REVISED VERSION OF THE GENERAL PURPOSE
MONTE CARLO PROGRAM, COHORT

VOLUME I - THEORY AND TECHNIQUES

By

N. R. Byrn

October 1969
(Revised April 1970)

Prepared For

NUCLEAR AND PLASMA PHYSICS DIVISION
SPACE SCIENCES LABORATORY
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ABSTRACT

CAVEAT (COHORT with Air Model, Variable Dimensioning, Energy Deposition, And Time Dependence) is a general purpose Monte Carlo computer code for neutron, gamma, and secondary gamma radiation transport calculations. This volume describes the mathematical concepts used in CAVEAT and the computational techniques that are applied in solving radiation transport problems. The code is written in the FORTRAN IV language and has been run on the IBM 7094, IBM 360, and UNIVAC 1108 computers. CAVEAT is a revised version of the COHORT program, with additional features such as time dependence, real atmosphere model, variable dimensioning, and, for third generation computers, a pass option which allows complete execution of a given problem, from source particle generation to fluence calculation.

Approved:



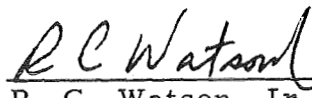
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1. INTRODUCTION

CAVEAT is a revised version of the general purpose Monte Carlo computer code, COHORT (Refs. 1 and 2), and can be used to solve a wide range of radiation transport problems. The name, CAVEAT, is an acronym for COHORT with Air model, Variable dimensioning, Energy dependence, And Time dependence. CAVEAT, which is written in the FORTRAN IV language, contains all of the COHORT capabilities except for the low energy neutron scattering by materials option, and has the following features:

- Variable dimensioning
- Real atmosphere (air) model
- Time dependence
- Pass option.

The variable dimensioning feature was added to optimize the use of available core storage by computing the dimensions of arrays at execution time, instead of having fixed dimensions on all arrays. As a result, the restrictions on the number of elements, materials, regions, boundaries, energy data point, etc., have been removed and the only restriction now is due to core storage capability.

The air model and time dependence features were added to permit the solution of the nuclear weapons radiation transport problem. The atmosphere is described by 233 layers of air, each being 2 kilometers thick, in which the density varies exponentially. The data for the air model is the same as that used by the AIRTRANS code (Ref. 3), based on the 1962 Standard Atmosphere Model (Ref. 4). However, other air model data can be used, if desired, since the data are input quantities. The time dependent feature has been included by assigning each source particle a time of birth and then computing the age of the particle at each collision point.

CAVEAT, like its predecessors, consists of a family of routines, where each routine is run as a separate FORTRAN job, and usually more than one routine is needed to solve a given problem. To eliminate the requirement of having to make more than one run to obtain the desired results, a pass option has been included in CAVEAT for the third generation computer. With this option, the data generated by a routine for input into another routine is stored on a data file* and can be taken from this data file instead of from cards. Thus, using IBM 360 terminology, each CAVEAT routine can be run as a job step in a job that will solve a radiation transport problem, from source generation to final analysis. This pass option feature normally cannot be used on second generation computers such as the IBM-7094.

The features discussed above were included in CAVEAT to extend and improve the capabilities of this computational scheme to solve radiation transport problems. At the same time, an intense effort has been made to locate and correct all programming and physics errors in both the original version and the added features. Also, data handling has been simplified by eliminating the requirement for identifying and sequencing each data card and by creating cross section data files that can be used in other CAVEAT routines.

The techniques used in CAVEAT to perform radiation transport calculations are discussed in this volume, Volume I. The different techniques explained include

- Source generation
- Geometry description and calculations
- Nuclear data definitions
- Collision calculations
- Analysis.

* The term "data file" refers to data recording media such as magnetic tape, disk, or drum.

The input data for each of the CAVEAT routines is described in Volume II, the Users' Manual, which also describes briefly the different routines and suggestions on the proper use of CAVEAT. After the code user becomes familiar with the CAVEAT code, he will find that problem input data can be prepared with the aid of Volume II, with only infrequent reference to Volume I.

Preliminary calculations (Ref. 5) have been performed for the first two benchmark problems. These problems are prepared by the Benchmark Problems Group of the American Nuclear Society (ANS-6) Standards Committee (Ref. 6), which is sponsored by the Shielding and Dosimetry Division of the American Nuclear Society. These calculations are presented, as examples of the input and output data for CAVEAT and as verification of the CAVEAT computational techniques.

CAVEAT is an improved version of a Monte Carlo computer code that was first envisioned at the George C. Marshall Space Flight Center (MSFC), Huntsville, Alabama, in 1960. At that time, several aerospace companies with nuclear capabilities were requested to submit proposals for a Monte Carlo computer code capable of calculating the radiation environment and nuclear energy deposition within a complex geometry system such as a nuclear rocket stage. The original contract was awarded to General Dynamics/Fort Worth (then known as Convair). The first version of the code was published in 1962 (Ref. 7), and about a year later a revised version was published (Ref. 2), in which the code was called COHORT. In 1966, another improved version of COHORT was distributed by Radiation Research Associates, Inc., of Fort Worth. Many of the improvements in this version were made at the National Aeronautics and Space Administration's (NASA's) Lewis Research Center in Cleveland, Ohio. Since 1966, major improvements and modifications to COHORT have been made at Lewis Research Center and at Brown Engineering. The Lewis Research Center version is called COHORT-II (Ref. 8), and the original family of routines structure has been integrated

into one package. The Brown Engineering version retains the family of routines structure but incorporates the other features previously discussed. Because of the differences in approach between the Brown Engineering version and COHORT-II, the Brown Engineering version of the COHORT code is called CAVEAT, since a name such as COHORT-III would imply that it is a revision of COHORT-II.

The authors wish to acknowledge the assistance of those who have contributed to the development of the CAVEAT version of the COHORT code. Messrs. D. G. Collins and M. B. Wells of Radiation Research Associates, Inc., were very helpful, explaining many of the programming techniques and helping make many of the initial improvements. Both participated in the development and coding of the original COHORT. Mr. T. W. DeVries of General Dynamics/Fort Worth is another code originator who has contributed to CAVEAT, especially by informing the authors of programming errors in the original version.* The authors would like to thank Messrs. Lester C. Clemons, Jr., and Leonard Soffer of Lewis Research Center for the many interesting discussions on how they were improving the original version and on errors they had detected. Thanks are also given to Mr. Henry E. Stern of Space Sciences Laboratory at MSFC, who was the technical monitor for this modification of COHORT and who provided the technical guidance for many of the changes incorporated into CAVEAT.

* Because much of the text of this documentation of the CAVEAT code, like all previous documentations of modifications to the initial program (Refs. 1 and 2), is very similar to the original text (Ref. 7), a special thanks is extended to the authors of the original documentation, Messrs. M. B. Wells and C. F. Malone.

2. SOURCE GENERATION

CAVEAT has two routines, S01 and S02, for generating the 10 parameters that describe each source particle. The S01 routine generates the data necessary to define source neutrons and primary gammas, and S02 generates data for defining secondary gammas. The 10 parameters specified are the spatial coordinates X, Y, and Z; the direction cosines, A, B, and C; the initial energy E; the initial weight W; the initial age (or time) T; and the geometrical region of the source, NRI. This data is written on a data file in a format of 14 sets of the 10 parameters per record, except for the first and last record. The first record written on the data file is a bookkeeping record, which includes the source tape number and type of particles. The last record is a source data record, but may contain less than 14 sets of parameters. The total number of source particles that can be generated depends on the number of source records that physically can be written on the data file.

2.1 PRIMARY SOURCE PARTICLE ROUTINE, S01

The basic assumption for generating primary source particles by S01 is that the spatial, angular direction, energy, and time distributions are independent. This means that the discrete probability tables used in S01 consist of a set of values of an independent random variable and the corresponding probabilities. If $f(x)$ is the density function for x , then

$$\int_{x_i}^{x_{i+1}} f(x) dx = p_i$$

represents the probability that x lies between x_i and x_{i+1} . Random values of x_i can be chosen from the cumulative probability distribution defined by determining the smallest value of i for which

$$\sum_{j=1}^i p_j \geq R_1 \quad ,$$

where R_1 is a number selected at random from a uniform distribution between zero and one (hereafter referred to as a random number). The actual value of x will be determined by choosing another random number, R_2 , and computing

$$x = x_i + R_2 (x_{i+1} - x_i) \quad .$$

The number and types of discrete probability tables required for input in S01 are determined by the options used in selecting the source parameters. These options are explained in detail in the following sections. All capital R's with subscripts represent random numbers.

2.1.1 Spatial Coordinate Options

The control parameter, IC, is used to specify the method of selecting the particle's spatial coordinates. The H01 routine has the capability of translating these coordinates, and, therefore, the center of the source region can be placed at the origin of the coordinate axes to simplify spatial coordinate generation. The different spatial coordinates options are discussed below.

- IC = 0: Point Source. The source is located at the origin of the coordinate system, i. e., $X = 0$, $Y = 0$, $Z = 0$.
- IC = 1: Rectangular Volume, Area, or Line Source. It is assumed that the source density, i. e., the source per unit volume, area, or length, as the case may be, is known, and that the source can be divided into smaller subregions, e. g., subvolumes for the rectangular volume source and line segments for the line source. The probability, p_i , represents the fraction of the total source density to be assigned to the i th subregion, with sides defined by $X(i, \text{min})$, $X(i, \text{max})$;

$Y(i, \min), Y(i, \max); Z(i, \min), Z(i, \max)$. For rectangular area sources, one set of min and max sides are set equal to each other, depending on the orientation of the area. For line sources, two sets of min and max sides have the min side equal to the max side.

The subregion in which the particle is to be generated is chosen by computing the smallest value of i , for which

$$\sum_{j=1}^i p_j - R_1 \geq 0 \quad .$$

The coordinates of the source point are then given by

$$X = X_{(i, \min)} + R_2 \left[X_{(i, \max)} - X_{(i, \min)} \right]$$

$$Y = Y_{(i, \min)} + R_3 \left[Y_{(i, \max)} - Y_{(i, \min)} \right]$$

$$Z = Z_{(i, \min)} + R_4 \left[Z_{(i, \max)} - Z_{(i, \min)} \right]$$

Hence, for a rectangular area source; say in the X-Y plane, $Z(i, \min)$ would equal $Z(i, \max)$, so that all values of Z would be the same.

- IC = 2; Spherical Volume Source. It is assumed that the total source distribution is known and that the distribution is dependent only on the radial distance, r , from the center of the sphere. The quantities, p_i , are defined as the source densities in the spherical shell volumes located between radii, r_i , and r_{i+1} .

The spherical shell volume, in which the particle is to be started, is chosen by computing the smallest value of i , for which

$$\sum_{j=1}^i p_j - R_1 \geq 0 \quad .$$

The coordinates of the source point are then determined by choosing a radius, r , where

$$r = [r_i^3 + R_1 (r_{i+1}^3 - r_i^3)]^{\frac{1}{3}} \quad .$$

Hence, the source in each spherical shell is assumed to be uniform. Using the radius chosen above, the spatial coordinates are chosen as

$$X = \left(\frac{2 R_3 - 1}{a} \right) r \quad ,$$

$$Y = \left(\frac{2 R_4 - 1}{a} \right) r \quad ,$$

and

$$Z = \left(\frac{2 R_5 - 1}{a} \right) r \quad ,$$

where $a^2 = (2 R_3 - 1)^2 + (2 R_4 - 1)^2 + (2 R_5 - 1)^2 \leq 1$.

- IC = 3: Cylindrical Volume Source. It is assumed that the source distribution can be separated into two distributions, one distribution along the Z axis and a radial distribution. Tables giving the distribution of p as a function of Z and the distribution of q as a function of r are required as program input.

Values for i and j are determined by computing the smallest values of i and j, for which

$$\sum_{n=1}^i p_n - R_1 \geq 0$$

and

$$\sum_{k=1}^i p_k - R_2 \geq 0 \quad .$$

Values for r and Z are then computed by using the equations

$$r = [r_j^2 + R_3 (r_{j+1}^2 - r_j^2)]^{\frac{1}{2}}$$

and

$$Z = Z_i + R_4 (Z_{i+1} - Z_i) \quad .$$

The source point coordinates for X and Y are determined from the equations

$$X = \left(\frac{2 R_5 - 1}{b} \right) r$$

and

$$Y = \left(\frac{2 R_6 - 1}{b} \right) r \quad ,$$

where $b^2 = (2 R_5 - 1)^2 + (2 R_6 - 1)^2 \leq 1$.

- IC = 4: Z-Plane Disk Surface Source. The source approximates a disk surface located in a plane normal to the Z axis. It is assumed that the source can be defined in terms of the probability, p_i , that a particle will be born in the area located between r_i and r_{i+1} . The area from which the particle is to be started is determined by computing the smallest i , for which

$$\sum_{j=1}^i p_j - R_1 \geq 0 \quad .$$

The X and Y coordinates of a source particle are computed by use of the equations

$$X = \left(\frac{2 R_3 - 1}{b} \right) r$$

and

$$Y = \left(\frac{2 R_4 - 1}{b} \right) r \quad ,$$

where $r = [r_i^2 + R_2 (r_{i+1}^2 - r_i^2)]^{\frac{1}{2}}$ and

$$b^2 = (2 R_3 - 1)^2 + (2 R_4 - 1)^2 \leq 1 \quad .$$

A table giving the distribution of p as a function of r is required as program input.

- IC = 5: Spherical Surface Source. The source approximates a spherical surface in which all the source particles are leaving the surface of the sphere in directions defined by the angular distribution of a point source located at the center of the sphere. The point source description assumes that the angular distribution of the leakage can be expressed in terms of only the polar angle, θ , about the positive Z axis.

The quantity, p_i , is defined as the fraction of the total leakage from the spherical surface that leaks out between θ_i and θ_{i+1} . The polar angle interval, through which the particle is leaving the surface, is determined by computing the smallest i , for which

$$\sum_{j=1}^i p_j - R_1 \geq 0 \quad .$$

The polar angle, θ , is then determined from

$$\theta = \theta_i + R_2 (\theta_{i+1} - \theta_i) \quad .$$

The spatial coordinates, from which the source particle leaves the surface, are given by

$$Z = r \cos \theta \quad ,$$

$$X = (r^2 - Z^2)^{\frac{1}{2}} \cos \phi \quad ,$$

and

$$Y = (r^2 - Z^2)^{\frac{1}{2}} \sin \phi ,$$

where r is the radius of the sphere, ϕ is the azimuthal angle assumed to be uniformly distributed, and

$$\cos \phi = \frac{(2 R_3 - 1)}{[(2 R_3 - 1)^2 + (2 R_4 - 1)^2]^{\frac{1}{2}}}$$

and

$$\sin \phi = \frac{(2 R_4 - 1)}{[(2 R_3 - 1)^2 + (2 R_4 - 1)^2]^{\frac{1}{2}}} ,$$

where $(2 R_3 - 1)^2 + (2 R_4 - 1)^2 \leq 1$.

The direction cosines of the source particle are given by

$$\alpha = \sin \theta \cos \phi ,$$

$$\beta = \sin \theta \sin \phi ,$$

and

$$\gamma = \cos \theta .$$

Tables giving the distribution of p as a function of θ and r are required as program input.

- IC = 6: Cylindrical Surface Source. The source approximates a cylindrical surface from which the angular distribution of the leakage is defined in terms of a point source dependent only on the polar angle θ . The angular interval, through which the particle leaves the source, is determined by computing the smallest value of i , for which

$$\sum_{j=1}^i p_j - R_1 \geq 0 \quad .$$

The polar angle, θ , is then computed from

$$\theta = \theta_i + R_2 (\theta_{i+1} - \theta_i) \quad .$$

The quantities $\theta_{\min}$ and $\theta_{\max}$, are defined as the minimum and maximum polar angles through which the source particles can leak out of the sides of the cylinder. The points, Z_1 and Z_2 , are defined as the Z coordinates of the planes bounding the ends of the cylinder. If $\theta \geq \theta_{\max}$, then $Z = Z_1$. If $\theta \leq \theta_{\min}$, then $Z = Z_2$. If $\theta_{\min} < \theta < \theta_{\max}$, Z is given by $Z = r \cot \theta$, where r is the radius of the cylinder. The X and Y coordinates of the source point are computed from the equations

$$X = Z \tan \theta \cos \phi$$

and

$$Y = Z \tan \theta \sin \phi \quad ,$$

where $\sin \phi$, $\cos \phi$, and the direction cosines α , β , and γ are defined as in IC = 5.

Tables giving the distribution of p as a function of θ , along with the quantities $\theta_{\min}$, $\theta_{\max}$, Z_1 , Z_2 , and r, are required as input to the program.

It should be noted that when IC = 5 or IC = 6 the distribution for the initial directions of motion also defines the initial spatial locations of the particles.

2.1.2 Direction Cosines Options

The S01 routines allow 10 different methods of selecting the particle direction cosines. The particular methods chosen are determined by the control parameter, ID, and are described below.

- ID = 0: Direction Cosines. The direction cosines are defined in the method used to generate spatial coordinates when IC = 5 or IC = 6.

- ID = 1: Constant Particle Direction. All particles leave the source with direction cosines, α , β , and γ , as specified in the program input. No probability tables are required as program input.
- ID = 2: Isotropic Source. No probability distribution tables are required. The direction cosines are determined by use of a rejection technique illustrated in Figure 2-1 and may assume random values between +1 and -1.
- ID = 3: Anisotropic Source (θ -dependent). This option provides a method of choosing random direction cosines, where the cosine of the polar angle, θ , is defined by a probability table and where the azimuthal angle, ϕ , is assumed to be uniformly distributed between 0 and 2π .

If h_i represents the probability that the cosine of the polar angle lies between γ_i and γ_{i+1} , then i can be computed by determining the smallest value of i , for which

$$\sum_{j=1}^i h_j - R_1 \geq 0 \quad .$$

The direction cosine, γ , is then given by

$$\gamma = \gamma_i + R_2 (\gamma_{i+1} - \gamma_i) \quad .$$

The direction cosines, α and β , are determined by first generating two random numbers, R_3 and R_4 , for which

$$b^2 = (2 R_3 - 1)^2 + (2 R_4 - 1)^2 \leq 1 \quad ,$$

and then evaluating equations

$$\alpha = \left(\frac{2 R_3 - 1}{b} \right) (1 - \gamma^2)^{\frac{1}{2}}$$

and

$$\beta = \left(\frac{2 R_4 - 1}{b} \right) (1 - \gamma^2)^{\frac{1}{2}} \quad .$$

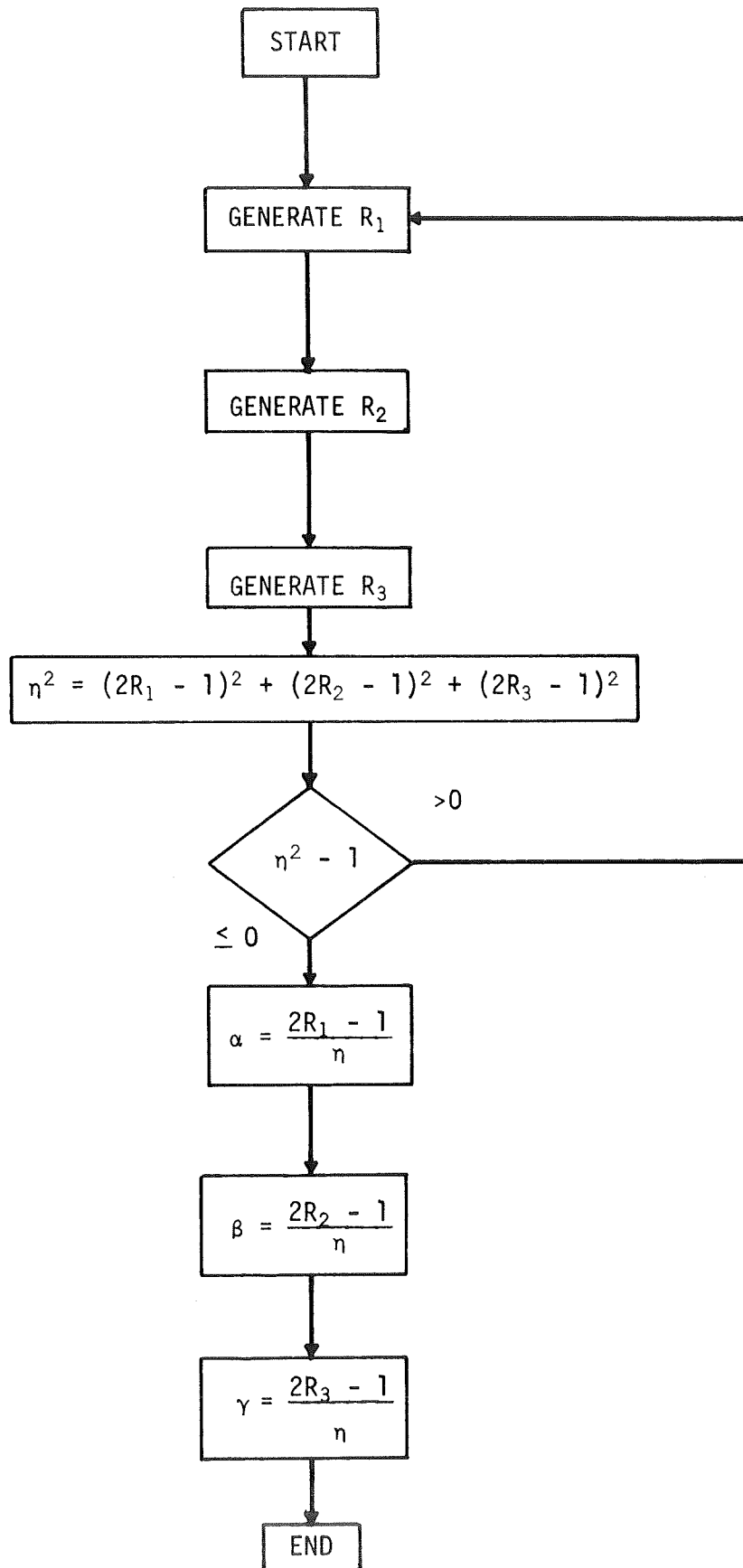


FIGURE 2-1. SELECTION OF RANDOM DIRECTION COSINE IN THE LABORATORY SYSTEM

Tables giving the distribution of h as a function of the direction cosine, γ , are required as program input.

- ID = 4: Anisotropic Source (θ - and ϕ -Dependent). It is assumed that the angular distribution can be divided into a distribution for the cosine of the polar angle, θ , and a distribution for the azimuthal angle, ϕ , as a function of the angle θ . The variable, h_i , is defined as the probability that θ lies in the interval, $\theta_i - \theta_{i+1}$. The distribution, $q_{i,j}$, is defined as the probability that source particles leaving the i th interval of θ will have directions defined by an angle, ϕ , that lies in the j th interval of the azimuthal angle, ϕ .

The polar angle interval is determined by computing the smallest value of i , for which

$$\sum_{\ell=1}^i h_{\ell} - R_1 \geq 0 \quad ,$$

and then computing the smallest value of j , for which

$$\sum_{m=1}^j q_{i,m} - R_2 \geq 0 \quad ,$$

where i is the interval of θ selected above.

The direction cosine, γ , and the angle, ϕ , are then computed by use of the equations

$$\gamma = \gamma_i + R_3 (\gamma_{i+1} - \gamma_i)$$

and

$$\phi = \phi_{i,j} + R_4 (\phi_{i,j+1} - \phi_{i,j}) \quad .$$

The direction cosines, α and β , are then given by

$$\alpha = \cos \phi (1 - \gamma^2)^{\frac{1}{2}}$$

and

$$\beta = \sin \phi (1 - \gamma^2)^{\frac{1}{2}} \quad .$$

Tables giving the distributions of h and q as a function of the direction cosine, γ , and the azimuthal angle, ϕ , are required as program input.

- ID = 5: Isotropic Source - Positive X Direction. The direction cosines are chosen in the same manner as that described for option ID = 2, but the direction cosine, α , is always taken as positive. No probability tables are required for this option.
- ID = 6: Isotropic Source - Negative X Direction. The direction cosines are chosen in the same manner as that described for option ID = 2, with the exception that the direction cosine, α , is always taken as negative. No probability tables are required for this option.
- ID = 7: Isotropic Source - Positive Y Direction. The method used to choose the direction cosines is the same as that described for option ID = 2, with the exception that the direction cosine, β , is always taken as positive. No probability input tables are required for this option.
- ID = 8: Isotropic Source - Negative Y Direction. The method used to choose the direction cosines is the same as that described for option ID = 2, with the exception that the direction cosine, β , is always taken as negative. No probability input tables are required for this option.
- ID = 9: Isotropic Source - Positive Z Direction. The method used to choose direction cosines is the same as that described for option ID = 2, with the exception that the direction cosine, γ , is always taken as positive. No probability input tables are required for this option.
- ID = 10: Isotropic Source - Negative Z Direction. The method used to choose the direction cosines is the same as the described for option ID = 2, with the exception that the direction cosine, γ , is always taken as negative. No probability input tables are required for this option.

2.1.3 Energy Option

A control parameter, IE, is used to determine the method of selecting the initial energy of each source particle. The various methods are described below.

- IE = 1: Constant Energy. This option provides a method of starting all source particles with the same initial energy. When this option is used, the initial energy, E, is entered as input in the program.
- IE = 2: Variable Energy. This option provides a method of selecting source energies from a continuous energy spectrum. The probability that a source particle will be emitted in the ith energy interval is denoted by p_i . A random value of i is determined by computing the smallest value of i, for which

$$\sum_{j=1}^i p_j - R_1 \geq 0 \quad .$$

The initial energy assigned the particle is computed from the equation

$$E = E_i + R_2 (E_{i+1} - E_i) \quad ,$$

where E_i is the lower bound of the ith energy interval. A table giving the distribution of p as a function of the energy, E, is required as program input.

The energy units for E or E_i can be either MeV, KeV, or eV, but the units must be consistent throughout a given CAVEAT problem.

2.1.4 Time Option

One of the features of CAVEAT not included in previous versions of COHORT is time dependence. Two methods are available in S01 for determining the time of birth (or age) of source particles. The methods used are determined by the input control parameter, IT, and are described below.

- IT = 1: Fixed Time of Birth. This method generates all source particle with an age of T, as specified in the problem data input.
- IT = 2: Time Spectrum: This method allows the input of the discrete cumulative distribution function of specified time intervals. If P_i is the discrete cumulative distribution function

through the i th time interval, then the interval in which a source particle is generated is selected by determining the smallest value of i , for which

$$P_i \geq R_1 \quad .$$

The initial age (or time of birth) of the particle is then computed by

$$T = T_i + R_2 (T_{i+1} - T_i) \quad ,$$

where T_i and T_{i+1} are, respectively, the lower and upper times on the i th time interval.

The time units for the age must be in seconds, since all time calculations in the history routine are in seconds.

2.2 SECONDARY GAMMA SOURCE ROUTINE, S02

The CAVEAT code has the capability of generating secondary gammas from a variety of reactions through the S02 routine. Although the discussion below uses the inelastic, (n, n') , process to illustrate the method used to generate secondary gammas, any of the other gamma producing reactions can be considered. These reactions also include (n, γ) , (n, α) , (n, p) , and combinations thereof. The S02 routine is programmed so that two different reaction types, or combinations, can be run at the same time, producing a data file for each. Because of historical reasons, these two service files are referred to as the inelastic and capture files. However, this does not mean that the use is restricted to generating secondary gammas from inelastic or capture events only. For example, secondary gammas generated by events which include (n, n') , (n, p) , and (n, α) could be placed on either the inelastic or the capture data file, depending on the way in which the input data is given to the routine. In fact, secondary gammas from inelastic events could be stored on the capture data file, if desired. However, since, in most cases, secondary gamma are produced by inelastic and/or capture

events, the secondary gamma will normally be stored on the appropriately named data file.

The input to S02 includes a data file containing the collision parameters generated during a neutron history calculation by the H01 routine. From each set of collision parameters, the spatial coordinates, energy, weight, age, and collision regions are extracted. Even though the element with which the collision took place is known, S02 ignores this data because secondary gammas are generated on a "material" basis, not on an element basis, as described below.

If a neutron with energy E_j has undergone a collision in a region containing material M then the probability $P_M(E_j)$ that the collision is an inelastic scattering event is defined by the expression

$$P_M(E_j) = \frac{\sum_{i=1}^{NE} N_{M,i} \sigma_{i,n,n'}(E_j)}{\sum_{i=1}^{NE} N_{M,i} \sigma_{i,T}(E_j)},$$

where

- NE - the number of elements required to describe the materials contained in a given problem
- $N_{M,i}$ - the atomic density of element i in material M
- $\sigma_{i,n,n'}(E_j)$ - the microscopic inelastic scattering cross section for element i at energy E_j
- $\sigma_{i,T}(E_j)$ - the microscopic total cross section for element i at energy E_j .

S02 computes the probability $P_M(E_j)$ from the elemental densities and cross section data input to the routine. Likewise, two other material quantities are computed from elemental data.

The quantity $\nu_M(E_j)$ is denoted as the average number of gamma rays emitted for each inelastic scattering event at the neutron energy E_j in material M and is defined by

$$\nu_M(E_j) = \frac{\sum_{i=1}^{NE} N_{M,i} \sigma_{i,n,n'}(E_j) \nu_i(E_j)}{\sum_{i=1}^{NE} N_{M,i} \sigma_{i,n,n'}(E_j)},$$

where $\nu_i(E_j)$ is defined as the average number of gamma rays given off after an inelastic collision with element i, and a neutron with energy E_j .

The quantity $q_{M,j,k}$ is denoted as the probability that a gamma ray with energy E_k will be given off after an inelastic collision in material M of a neutron with energy E_j and is defined as follows:

$$q_{M,j,k} = \frac{\sum_{i=1}^{NE} N_{M,i} \sigma_{i,n,n'}(E_j) \nu_i(E_j)}{\sum_{i=1}^{NE} N_{M,i} \sigma_{i,n,n'}(E_j)},$$

where $q_{i,j,k}$ is defined as the probability that a gamma ray with energy E_k will be given off following an inelastic collision with element i by a neutron with energy E_j .

Similar quantities, P_M , ν_M , and $q_{M,j,k}$, are defined for other reaction types and/or combination of reaction types.

A program option, called IOP_i, is used to indicate the method by which gamma rays are to be generated for a particular type of event in a given material. The index on IOP is determined by specifying that all odd integers represent the events whose secondary gammas are to be written on the inelastic data files, and all even integers represent the

events where secondary gammas are to be written on the capture data file. Then the indexes for the IOP for the Nth material is $2*N-1$ and $2*N$. For the event and material, M, that correspond to the index I, if

- IOP(I) = 0: Secondary gammas are produced only for those collisions in which

$$P_M(E) \geq R \quad ,$$

where R is a random number.

The weight of the secondary gamma is computed by

$$W_\gamma = W \nu_M(E) \quad ,$$

where

W - the neutron weight before collision

E - the neutron energy before collision.

- IOP(I) = 1: A secondary gamma is produced at energy collision for which the neutron energy falls within the event energy range. The secondary gamma weight is computed by

$$W_\gamma = W \nu_M(E) P_M(E) \quad .$$

This weight is then compared with certain input quantities to determine whether it should be stored on the proper secondary gamma data file.

Unlike previous versions of COHORT, all secondary gammas generated when IOP(I) = 1 are not necessarily used as sources. Instead, the secondary gammas are characterized by weight, with those gammas whose weight exceed a certain value accepted as sources. Those gammas that fall below this value are placed into one of two weight categories, and are required to play Russian Roulette successfully in order to become sources.

Whenever a secondary gamma source is generated at any collision point, the 10 parameters that specify that source are then determined.

The spatial coordinates, age, and source region are the same as that of the neutron at collision. The angular distribution of the initial direction of the secondary gamma is assumed to be isotropic in the laboratory system. The initial direction cosines, A, B, and C, are chosen at random by using the rejection technique illustrated in Figure 2-1.

The initial energy of the secondary gamma is determined by computing the smallest value of k, for which

$$\sum_{\ell=1}^k q_{M,j,\ell} \geq R \quad ,$$

where R is a random number. The energy is then taken to be equal to the kth entry in the table of gamma energies input for the jth incident neutron energy group. The j that is used to look up the values of $q_{M,j,\ell}$ in the above expression is that value of j for which the neutron energy, E_n , satisfies the equation

$$E_j \leq E_n \leq E_{j+1} \quad .$$

Finally, the weight of the secondary gamma is that weight computed above for the appropriate value of IOP, except when the gammas successfully play Russian Roulette. For these gammas, the initial gamma weight is divided by the Russian Roulette parameter.

3. GEOMETRY DESCRIPTION AND CALCULATIONS

For Monte Carlo codes such as CAVEAT, which allow the tracking of particles through complex geometries, a procedure is needed so that the code can determine the location of a particle relative to the problem geometry. The procedure used by CAVEAT consists of describing the problem geometry by defining various linear and quadratic surfaces which bound geometric regions. The region a particle is in is determined by calculating its position relative to the bounding surfaces, or boundaries, of each region. The distance to boundaries are computed by analytical geometry techniques. This section discusses the geometry procedure used by the history (H01) and analysis (A01 and A02) routines.

3.1 GEOMETRY DESCRIPTION

The geometry description of a given problem is accomplished by describing the boundaries of regions by equations of surfaces of revolution about the Z axis or about lines parallel to the Z axis and by equations of planes normal to the X, Y, Z coordinate axes or planes inclined at an angle, θ , to the X axis. Inside regions are those geometric regions which are completely bounded by surfaces. Only one outside region is allowed, and it must always be designated as region 2. This region consists of all space outside of the problem geometry.

To simplify the input describing the geometry, eight special cases of boundaries are available. A code number, IBT(K), is used to specify which of the eight equations is to be used and which parameters are required for each of the K boundaries. The code numbers have the following meaning:

- IBT(K) = 1: $(X - XF)^2 + (Y - YF)^2 - AF(Z - ZF)^2 - CF = 0$
- IBT(K) = 2: $(X - XF)^2 + (Y - YF)^2 - AF(Z - ZF) = 0$

- IBT(K) = 3: $[(X - XF)^2 + (Y - YF)^2]^{\frac{1}{2}} - AF(Z - ZF) = 0$
- IBT(K) = 4: $[(X - XF)^2 + (Y - YF)^2]^{\frac{1}{2}} - AF = 0$
- IBT(K) = 5: $\theta - AF = 0$
- IBT(K) = 6: $Z - AF = 0$
- IBT(K) = 7: $X - AF = 0$
- IBT(K) = 8: $Y - AF = 0$
- IBT(K) = 9: $AF \cdot X + ZF \cdot Y + CF \cdot Z - XF = 0,$

where AF, ZF, CF, XF, and YF are input parameters. Only those parameters necessary to define the selected equation, along with the code number, are entered as input. Code numbers 1 through 4 define surfaces in terms of the rectangular coordinates, X, Y, and Z.

The surface of revolution defined by revolving Equation 1 about a line parallel to the Z axis will be either an ellipsoid, hyperboloid, or a sphere. Those obtained by revolving code numbers 2, 3, and 4 about a line parallel to the Z axis are paraboloids, cones, and cylinders, respectively. Code number 5 represents a plane passing through the Z axis inclined at an angle AF to the X axis. Code numbers 6, 7, and 8 represent planes normal to the coordinate axes listed, and code number 9 represents an arbitrarily oriented plane. The units of AF, ZF, CF, XF, and YF are in centimeters for all equations except code number 5. In code number 5, AF is in radians.

3.2 GEOMETRY CALCULATIONS

The geometry calculations consist of computing the distance from a source point or collision point to a boundary of the region containing the point, determining the region entered when the particle crosses a boundary, and computing the distance to collision.

3.2.1 Distance to Boundary

The equation giving the straight-line distance from a particle's position in a region to a boundary of the region is given by

$$S = \frac{-b \pm (b^2 - ac)^{\frac{1}{2}}}{a}$$

for boundaries for which the code number IBT(K) has a value of 1, 2, 3, or 4. The parameters, a, b, and c, are dependent on the value of IBT(K); the coordinates, X, Y, and Z, of the point; and the direction cosines, α , β , and γ , of the line. This dependency is demonstrated by the equations

- IBT(K) = 1: $a = \alpha^2 + \beta^2 - AF\gamma^2$
 $b = \alpha(X - XF) + \beta(Y - YF) - \gamma AF(Z - ZF)$
 $c = (X - XF)^2 + (Y - YF)^2 - AF(Z - ZF)^2 - CF$
- IBT(K) = 2: $a = \alpha^2 + \beta^2$
 $b = \alpha(X - XF) + \beta(Y - YF) - \frac{1}{2}\gamma AF$
 $c = (X - XF)^2 + (Y - YF)^2 - AF(Z - ZF),$
- IBT(K) = 3: $a = \alpha^2 + \beta^2 - (AF)^2 \gamma^2$
 $b = \alpha(X - XF) + \beta(Y - YF) - (AF)^2 \gamma (Z - ZF)$
 $c = (X - XF)^2 + (Y - YF)^2 - (AF)^2 (Z - ZF)^2$
- IBT(K) = 4: $a = \alpha^2 + \beta^2$
 $b = \alpha(X - XF) + \beta(Y - YF)$
 $c = (X - XF)^2 + (Y - FY)^2 - (AF)^2 .$

If $(b^2 - ac) < 0$, $a = 0$; or if b/a and c/a are both positive for any of the boundaries of the region, there are no intersections of the particle's path with these boundaries. The choice of the sign before the radical in the equation for S depends on the numerical values of the parameters, b/a and c/a . In all cases, the decision as to which sign is to be used is based on the fact that only positive values of S are of interest.

The distance, S , from a point inside a region to a boundary for which the code number $IBT(K)$ is 5, 6, 7, 8, or 9 is given by the equations

- $IBT(K) = 5: S = \frac{X \sin AF - Y \cos AF}{-\alpha \sin AF + \beta \cos AF}$
- $IBT(K) = 6: S = \frac{AF - Z}{\gamma}$
- $IBT(K) = 7: S = \frac{AF - X}{\alpha}$
- $IBT(K) = 8: S = \frac{AF - Y}{\beta}$
- $IBT(K) = 9: S = \frac{XF - X \cdot AF - Y \cdot ZF - Z \cdot CF}{\alpha \cdot AF + \beta \cdot ZF + \gamma \cdot CF}$.

A distance, S , is computed for each of the boundaries defining the region containing the particle. The smallest positive value of the S 's so computed is taken as the distance, S , to the region boundary.

After the distance to the boundary of the region has been determined, the coordinates of the intersection of the particle's path with the boundary are determined from the equations

$$X = X + \alpha S,$$

$$Y = Y + \beta S,$$

$$Z = Z + \gamma S,$$

where X, Y, and Z in the right-hand member of the equations are the particle's previous coordinates.

3.2.2 Region Containing the Particle

If the distance to collision is greater than the distance to the boundary of the region containing the particle, it is stepped across the boundary to the point represented by

$$X1 = Y + EPSL \cdot \alpha$$

$$Y1 = Y + EPSL \cdot \beta$$

$$Z1 = Z + EPSL \cdot \gamma ,$$

where EPSL is a small distance used to ensure that the particle is stepped across the boundary.

The library input contains a list of boundaries for each region and a list of the regions most probably entered if the particle crosses one of these boundaries. The code checks to see, when the particle crosses a boundary, whether it is in the region most likely to be entered. If it is not in that region, the code checks all the remaining regions until it finds the one entered. If the particle cannot be found within any region, an error comment is printed out and the history is terminated.

A region contains the particle only if the particle is in that region with respect to all boundaries of that region. Using the input parameters and the particle's spatial coordinates, X1, Y1, and Z1, a quantity, XR, is computed for each of the region boundaries by use of the following equations:

- $IBT(K) = 1: \quad XR = (X1 - XF)^2 + (Y1 - YF)^2 - AF(Z1 - ZF)^2 - CF$
- $IBT(K) = 2: \quad XR = (X1 - XF)^2 + (Y1 - YF)^2 - AF(Z1 - ZF)$
- $IBT(K) = 3: \quad XR = (X1 - XF)^2 + (Y1 - YF)^2 - (AF)^2 (Z1 - ZF)^2$
- $IBT(K) = 4: \quad XR = (X1 - XF)^2 + (Y1 - YF)^2 - (AF)^2$
- $IBT(K) = 5: \quad XR = (X1) \sin AF - (Y1) \cos AF$
- $IBT(K) = 6: \quad XR = Z1 - AF$
- $IBT(K) = 7: \quad XR = X1 - AF$
- $IBT(K) = 8: \quad XR = Y1 - AF$
- $IBT(K) = 9: \quad XR = X1 \cdot AF + Y1 \cdot ZF + Z1 \cdot CF - XF$

If XR is negative, the particle is on one side of the boundary; if $XR = 0$, the particle is on the boundary; and if XR is positive, the particle's position is on the other side of the boundary. Therefore, the quantity, XR , determines on which side of the boundary the particle is located.

The concept of "inner" and "outer" boundaries is used to determine whether the particle lies inside or outside a region. The inner boundary is defined as one for which the quantity, XR , will be positive with respect to the particle's position. An outer boundary is one for which the quantity, XR , will be negative with respect to the particle's position. Since a boundary may be an inner boundary for one region and an outer boundary for another region, a plus or a minus sign is attached to the boundary number of each region to specify the "inner" or "outer" region. The sign is chosen so that if the signs of the boundary number and XR are the same the particle is inside the region with respect to the boundary for which XR is computed. In order for the particle to be within the region, the sign of the boundary number and the parameter, XR , must be alike for all boundaries of the region.

4. NUCLEAR DATA FOR TRANSPORT CALCULATIONS

The Monte Carlo technique involves the mathematical simulation of the physical events occurring during transport of particles. Thus, in addition to the geometry of the problem, the nuclear properties must be described. These properties include the atomic weights and densities of materials, the nuclear cross sections, and inelastic scattering and anisotropic scattering data for neutrons.

Each geometric region of the problem geometry is assumed to consist of a homogeneous mixture of elements (and/or nuclides), which is called a material. The composition of each material is defined by specifying the density of the elements contained in the material. If any material contains more than one isotope of an element, with the isotopes having different cross sections, each isotope may be treated as if it were a different element. Each different material is assigned a natural number. Void regions can be defined by setting the "material" number to zero in the problem input data; hence, no densities need be entered to define voids. Because of the variable dimensioning feature of CAVEAT, there is no limit on the number of materials and elements for a given problem, except total core storage.

The nuclear cross sections are input by giving the necessary microscopic cross sections for each element at arbitrarily-spaced energy points. The energy points must be the same for every element. When a cross section is needed at a given energy, it is found by linear interpolation between the input energy points. Hence, proper selection of the energy points is essential. In order to conserve computer core storage, the cross sections may be partitioned into energy supergroups. The cross sections and other nuclear data for only one supergroup are placed in core at any given time, beginning with the supergroup with the highest energies. CAVEAT does the transport of all source

particles in a given supergroup and terminates transport of any particle whenever the energy of that particle is reduced below the minimum energy for the supergroup. At that time, the parameters of the particle are stored on a data file. After all particles are transported through that supergroup, the data for the next lower energy supergroup is placed in core storage. The stored data are then read from the data file, and the particles are transported for the lower supergroup.

4.1 NEUTRON CROSS SECTIONS AND NUCLEAR DATA

4.1.1 Neutron Cross Sections

For neutron problems, the microscopic cross sections required by the history generator routine, H01, are the total cross section, the total scattering cross section, and the elastic scattering cross section. The total scattering cross section is normally assumed to be the sum of the elastic and inelastic scattering cross sections. The difference between the total and the total scattering cross sections is assumed to be the absorption cross section, an absorption event being one in which no neutron leaves the event. In certain problems, reactions such as $(n, 2n)$ make this simple representation of the cross sections inadequate, thus requiring some adjustment of the cross sections to handle the situation. For the analysis routines, A01 and A02, only the total cross sections are required input. However, CAVEAT generates a data file in the H01 routine that can be used in the A01 and A02 routines.

4.1.2 Anisotropic Elastic Scattering Data

Angular distributions for neutron elastic scattering in the center-of-mass coordinate system are required by the H01 and A01 routines for each element I (except hydrogen) and for each energy supergroup in which the neutrons have energy about $ESI(I)$, the energy below which elastic scattering is isotropic in the center-of-mass system. The energy

supergroups are partitioned into energy groups, over which an average differential elastic scattering distribution can be found. The distribution is defined as

$$f(E_i, \mu) d\mu = \frac{\frac{d\sigma}{d\Omega}(E_i, \mu) d\mu}{\int_1^{-1} \frac{d\sigma}{d\Omega}(E_i, \mu) d\mu}$$

where

E_i - the energy group

μ - the cosine of the scattering angle in the center-of-mass system

$\frac{d\sigma}{d\Omega}$ - the differential elastic scattering cross section.

For each element, I, within a given energy supergroup, the total area under the distribution curve is partitioned into NEPI(I) equal areas. From this partition, the cosine, μ_j , is determined; μ_j is defined by

$$\frac{j}{NEPI(I)} = \int_1^{\mu_j} f(E_i, \mu) d\mu \quad \text{for } j = 1, 2, \dots, NEPI(I)$$

Hence, the probability that an elastically scattering neutron will be scattered into the interval from μ_{j-1} to μ_j ($\mu_0 = 1$) is just $1/NEPI(I)$. Therefore, the input data required to define the anisotropic elastic scattering of neutrons is just the cosines of the center-of-mass scattering angles, μ_j , which are functions of the energy group and element of scatter.

Since the angular distribution of neutron scattering in hydrogen is isotropic in the center-of-mass system for energies above ELOW, the energy below which the motion of the target nuclei are considered, no anisotropic scattering data are required for hydrogen.

4.1.3 Inelastic Scattering Data

The inelastic scattering required by the H01 routine of CAVEAT consists of inelastic scattering cumulative probability tables for each applicable element as a function of specified incident energy groups and excitation levels. The incident energy groups are functions of the element of scatter and the energy supergroups, so that the energy groups are a partition of the energy supergroups. The energy of a neutron, after inelastic scattering, is computed by using excitation levels chosen at random from the proper probability table.

Although the required input data are tabular, much of the available inelastic scattering data are in the form on continuum distributions. For these data, psuedo-excitation levels may be chosen and probabilities for exciting these levels computed by integrating over some energy interval which the psuedo-excitation level represents.

4.2 GAMMA CROSS SECTIONS

The only nuclear cross sections required by CAVEAT for primary and secondary gammas are the total cross section, pair production plus Compton scattering cross sections, and the Compton scattering cross section. While the H01 routine requires all of the above, the A01 and A02 routines require only the total cross section. The sum of the pair production and Compton scattering cross sections is taken as the total scattering cross section, while the difference between the total cross section and the total scattering cross section is assumed to be the photoelectric cross section. The photoelectric cross section is treated the same as an absorption cross section. No other nuclear data are required by CAVEAT for the transport of gammas.

5. COLLISION PROCESSES

The previous sections have discussed the generation of source particles, geometry descriptions and calculations, and required nuclear cross sections and data. Based on this background, this section explains the techniques used to compute the position at which source particles have collisions and to determine the result of that collision. Most of these techniques are programmed into a collision distance (COLDST) subroutine and a scattering (SCATR) subroutine in the H01 routine. However, other subroutines for special cases are included in H01.

Since all collisions are treated in H01 as scattering collisions, the weight of the particle emerging from a collision is computed as the product of the weight before collision and the probability that the collision was a scattering event. The weight after collision becomes

$$W' = W \frac{\sum_S (E)}{\sum_T (E)},$$

where

W - weight before collision

$\sum_S (E)$ - total scattering macroscopic cross section

$\sum_T (E)$ - total macroscopic cross section

E - energy before collision.

5.1 DISTANCE TO COLLISION

To determine the position at which a collision takes place, the number of mean free paths that the particle travels on its flight from the previous collision (or source point) to the next collision point is selected from the exponential density distribution:

$$f(\lambda) = \exp(-\lambda) \quad \text{for } \lambda \geq 0 ,$$

where

$$\lambda = X \sum_T (\text{mean free paths})$$

$$X = \text{distance}$$

$$\sum_T = \text{total macroscopic cross section of the material through which the flight takes place.}$$

If R is a random number, then a particular value of λ , say λ_1 , is found by solving for λ_1 in the equation

$$R = \int_0^{\lambda_1} \exp(-\lambda) d\lambda .$$

Knowing λ_1 , the random distance, D, is computed by taking

$$D = \frac{\lambda_1}{\sum_T} ,$$

where it has been assumed that $\sum_T$ is a constant through the flight. After D has been calculated, a check is made to determine whether the flight path is confined to one region, in which case the determination of the next collision location is straightforward. If the particle enters another region, the exit position of the particle from the first region is determined and the length of the path, S, in that region is computed.

The distance the particle can travel in the new region entered is computed by the equation

$$D' = (D - S) \frac{\sum_T(E)}{\sum_{T'}(E)} .$$

where $\sum_{T_1}(E)$ is the total macroscopic cross section at the particle energy, E , for the region entered, and $\sum_T(E)$ is the total macroscopic cross section for the region just crossed. If the distance, D' , is less than the distance across the region just entered, the collision is taken to have occurred within that region. If D' is greater than the distance across the region just entered, the process outlined above is repeated as often as necessary.

5.1.1 Exponential Transformation

In problems for which the quantities to be calculated depend on the successful penetration of the particles to a large number of mean free paths into the system, the exponential transformation can be used to increase the probability of success of the particle by varying the mean-free-path length as a function of the particles' direction of motion in a region. The mean-free-path length can be varied in any of the six directions, $\pm\alpha$, $\pm\beta$, $\pm\gamma$, path lengths can be chosen which are independent of direction, or particles can be forced toward a biasing point.

A code number, $NEXT(K)$, is entered in the library input for each of the K regions to define the manner in which the exponential transformation is to be used for each region. A pseudo total macroscopic cross section, $\bar{\sum}_T(E)$, for each region is computed by

$$\bar{\sum}_T(E) = \sum_T(E) [1 - XK * EXT] ,$$

where EXT is a region dependent number such that $0 \leq EXT < 1$, which partially determines the amount of biasing. The parameter, XK , is defined in terms of the code number, $NEXT(K)$, for each region, K , as follows:

<u>Code Number</u>	<u>Definition</u>
NEXT(K) = 1	XK = 0
NEXT(K) = 2	XK = 1
NEXT(K) = 3	XK = α
NEXT(K) = 4	XK = $-\alpha$
NEXT(K) = 5	XK = β
NEXT(K) = 6	XK = $-\beta$
NEXT(K) = 7	XK = γ
NEXT(K) = 8	XK = $-\gamma$
NEXT(K) = 9	XK = $\alpha * \alpha_B + \beta * \beta_B$ $+ \gamma * \gamma_B$

where α_B , β_B , and γ_B are the direction cosines of the collision point-to-bias point direction. These direction cosines are computed by the code.

The psuedo total across section, $\bar{\sum}_T(E)$, is used in place of the total cross section, $\sum_T(E)$, to compute random path lengths, when NEXT(K) is 2 or greater.

If the exponential transformation is performed in a region and it is found that the next collision has occurred in the region, the bias introduced in the particle weight by the use of the exponential transformation is removed by modifying the particle weight as follows:

$$W' = W \frac{\sum_T(E)}{\bar{\sum}_T(E)} \exp \left\{ -D \left[\sum_T(E) - \bar{\sum}_T(E) \right] \right\} .$$

If a boundary crossing has occurred, the bias introduced in the particle weight is removed by modifying the weight at the boundary by the equation

$$W' = W \exp \left\{ -S \left[\sum_T (E) - \bar{\sum}_T (E) \right] \right\} ,$$

where S is the distance traveled from the collision point to the boundary.

5.1.2 Real Atmosphere "Air" Model

CAVEAT has a feature which allows the transport of particles in air through an atmosphere, whose density is a continuously varying function of the altitude above the ground plane. The air model is defined at altitudes up to 466 kilometers. The data for this air model are the same as that for the AIRTRANS (Ref. 3) model, which is based on the "U.S. Standard Atmosphere - 1962" (Ref. 4). The atmosphere is divided into 233 equally-spaced regions by horizontal planes. At each of these horizontal planes, the amount of air above the plane, in g/cm², and the atmospheric density are specified. The atmospheric density is assumed to vary exponentially between the planes, so that it is possible to compute the amount of atmosphere, in g/cm², above any point. It is assumed that the ratio between the concentrations of different elements in the air does not vary with altitude. The composition of the atmosphere is expressed as concentrations, e. g., atoms/g of material. When the air model is used in a problem, one material is specified as the air, and this material is the material for the atmospheric region or regions, since more than one region can contain air in the problem of geometry description.

5.2 NEUTRON SCATTERING OPTIONS

The H01 routine of CAVEAT has three options for treating neutron scattering events. The particular option used is specified by the two input energy parameters, ETM and ELOW. The energy ranges in which the different scattering options are applied are given below for a neutron of energy, E:

- $E > ETM$ and $E > ELOW$ - Only high energy neutron scattering events occur.
- $ETM \leq E \leq ELOW$ - Neutron scattering is dependent upon the velocity of the target atom.
- $E < ETM$ - Neutron scattering is isotropic in the laboratory system, with no energy loss.

The last two options are for low energy (or thermal) neutrons.

A detailed description of the techniques used in these options is given in the next two subsections.

5.2.1 High Energy Scattering Events

Whenever the incident neutron energy is both greater than ELOW, the scattering event is treated as a high energy event, i. e., one in which the target atoms are assumed to be at rest. The following method is used to select scattering parameters. The element of collision is selected by determining the smallest value of i , for which

$$\frac{1}{\sum_{J, T} (E)} \sum_{K=1}^i [DN(J, K) \sigma_{K, T}(E)] \geq R,$$

where

- J - material number of material in which collision occurred
- K - element number
- $\sum_{J, T}(E)$ - total macroscopic cross section of material, J , at the collision energy, E
- $DN(J, K)$ - density of the J th element in the K th material
- $\sigma_{K, T}(E)$ - total microscopic cross section of element, K , at energy, E
- R - random number.

The parameter i indicates with which of the K elements the collision is assumed to have occurred. If the element of collision so selected is hydrogen, a special routine is used to select the scattering parameters. The hydrogen elastic scattering and the scattering cross sections are assumed to be identical with the total cross section, and the scattering probabilities are assumed to be isotropic in the center-of-mass system. A random scattering angle in the laboratory system is selected from the density function, $f(\cos \psi) = 2 \cos \psi$, in the following manner: Generate two random numbers, R_1 and R_2 . Take the largest of these random numbers as $\cos \psi$. The energy after the collision is then given by $E' = E \cos^2 \psi$. The proof that the random variable, $\cos \psi = \text{Max}(R_1, R_2)$, is a sample from the density function, $f(\cos \psi) = 2 \cos \psi$, is given by Kahn (Ref. 10).

If the collision is with some element other than hydrogen, the type of scattering event is selected by determining for the i th element, if the difference

$$\frac{\sigma_{i, \text{el}}(E)}{\sigma_{i, \text{s}}(E)} - R$$

is greater than zero. If it is, the event is taken as an elastic scattering collision. If the difference is less than or equal to zero, the event is taken to be an inelastic collision.

If the scattering event is an inelastic collision, an excitation energy, E_x , is selected from a probability distribution table which has been entered for the element of collision as a function of the incident neutron energy. The quantity,

$$B = 1 - \frac{(A - 1) * E_x}{A * E} ,$$

where A is the atomic weight ratio, is computed for future use in the calculations.

An input energy, $ESI(I)$, is entered for each of the I elements. If the neutron's incident energy is less than the value of $ESI(I)$ entered for the collision element, elastic scattering is assumed to be isotropic in the center-of-mass system. If the incident energy is greater than the value entered for the collision element, elastic scattering is assumed to be anisotropic in the center-of-mass system. The cosine of the polar scattering angle in the center-of-mass system is then determined from input cumulative probability distribution tables as a function of incident neutron energy and element number.

The scattering probabilities for inelastic scattering are assumed to be isotropic in the center-of-mass system for all elements. A random cosine in the center-of-mass system is computed from the equation, $\cos \lambda = 2R - 1$. The cosine of the center-of-mass scattering angle is converted to the cosine of the laboratory scattering angle by the equation

$$\cos \psi = \frac{1 + A(B)^{\frac{1}{2}} \cos \lambda}{[1 + A^2 B + 2 A(B)^{\frac{1}{2}} \cos \lambda]^{\frac{1}{2}}}$$

and the energy after collision is determined from the equation

$$E' = E \left[1 - \frac{2A}{(A+1)^2} - \frac{A^2}{(A+1)^2} (1 - B) + \frac{2A}{(A+1)^2} B^{\frac{1}{2}} \cos \lambda \right]$$

where $B = 1$ for elastic scattering.

The azimuthal scattering angle, ϕ , is selected from a uniform distribution in the interval of 0 to 2π .

The directional cosines of the neutron's flight path after collision are computed from a knowledge of the polar and azimuthal scattering angles, ψ and ϕ , in the laboratory system and from the direction

cosines, α , β , and γ , of the incident neutron in the fixed reference system. The direction cosines in the fixed reference system are computed as follows:

when $(1 - \gamma^2) \geq 0.0001$,

$$\alpha' = \left(\frac{\alpha \gamma \sin \psi \cos \phi - \beta \sin \psi \sin \phi}{(1 - \gamma^2)^{\frac{1}{2}}} \right) + \alpha \cos \psi$$

$$\beta' = \left(\frac{\alpha \sin \psi \sin \phi + \gamma \beta \sin \psi \cos \phi}{(1 - \gamma^2)^{\frac{1}{2}}} \right) + \beta \cos \psi$$

$$\gamma' = \gamma \cos \psi - (1 - \gamma^2)^{\frac{1}{2}} \sin \psi \cos \phi ;$$

when $(1 - \gamma^2) < 0.0001$,

$$\alpha' = \sin \psi \cos \phi ,$$

$$\beta' = \sin \psi \sin \phi , \quad \text{and}$$

$$\gamma' = \cos \psi .$$

5.2.2 Low Energy Scattering Events

When the incident neutron energy, E , is such that $ETM \leq E \leq ELow$, the method of treating neutron scattering is one which takes into account the effects of the thermal motion of the target atoms. The target atom, or element, is selected in the manner given for high energy scattering.

The treatment of the target velocities and collision mechanics is essentially the same as that used by Brown (Ref. 9). The probability, p , of a collision between a neutron with velocity, $\vec{v}_1$, and a target atom of velocity, $\vec{V}$, depends upon the relative velocity and the distribution, due to thermal motion, of the target atom velocities. It is assumed that the target atoms possess a Maxwellian distribution of velocities, $M(\vec{V})$, in the laboratory system and that the scattering cross section in the center-of-mass system is independent of the target velocity. This assumption results in the probability of a collision with a moderator atom being obtained by integrating over all possible target atom velocities.

$$\begin{aligned} \int p d\vec{V} &= \int_0^\infty |\vec{v}_1 - \vec{V}| M(\vec{V}) d\vec{V} \\ &= \frac{1}{\beta \sqrt{\pi}} \exp(-\beta^2 v_1^2) \left(\frac{1}{2\beta^2 v_1} + v_1 \right) \text{Erf}(\beta v_1) \end{aligned}$$

where

$$\beta^2 = \frac{A^*}{2kT}$$

A^* - effective mass of the target atom (in neutron masses)

kT - moderator temperature

v_1 - $|\vec{v}_1|$

$\text{Erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-y^2) dy$ - the error function.

The target speed, V , i. e., $|\vec{V}|$, must be chosen at random from equally weighted samples of this integral probability. Since the integral probability is complex and therefore difficult to decompose into equally weighted samples, the differential probability is dealt with instead. The

selection of V is accomplished by the rejection technique illustrated in Figure 5-1. An upper bound of the integrand is $v_1 + V$. Thus, an upper bound of the probability is

$$\begin{aligned} \int p_{\max} d\vec{V} &= v_1 \int M(V) d\vec{V} + \int V M(V) d\vec{V} \\ &= v_1 + \frac{2}{\sqrt{\pi}} \left(\frac{kT}{A^*} \right)^{\frac{1}{2}} = v_1 + I . \end{aligned}$$

A random number, R_1 , is generated to decide the selection of V .
If

$$R_1 \leq \frac{v_1}{v_1 + I} ,$$

a value of V is selected at random from the Maxwellian distribution. If

$$R_1 > \frac{v_1}{v_1 + I} ,$$

V is selected at random from a V -weighted Maxwellian distribution. Although the V so selected is representative of the upper bound probability, $p_{\max}$, the actual probability is more restrictive. The frequency with which each speed, V , is chosen is too great and should be reduced by the fraction by which $p_{\max}$ exceeds p . A second random number, R , is generated to test the choice of V . If

$$R_2 \leq \frac{|\vec{v}_1 - \vec{V}|}{v_1 + V} ,$$

V is accepted as the target speed; otherwise, the sample is rejected and the sampling process repeated.

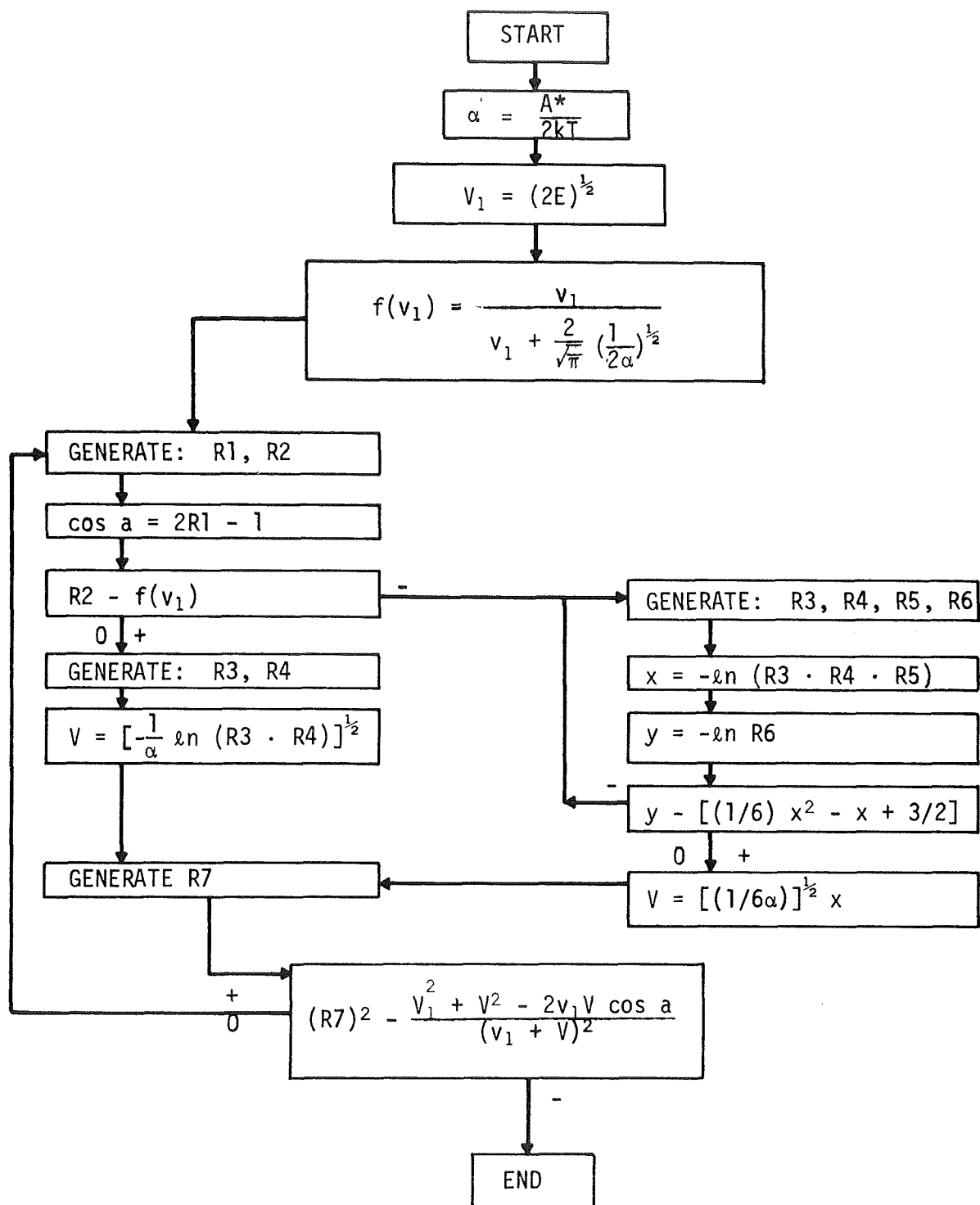


FIGURE 5-1. SELECTION OF TARGET VELOCITY FROM A MAXWELLIAN DISTRIBUTION

The rejection technique used to select samples from the Maxwellian and V-weighted Maxwellian distribution is credited to Kahn (Ref. 10). The direction of the target atom is assumed to be isotropic in the laboratory system, and a random angle, a , between the target atom and the neutron is selected from a cosine distribution.

The neutron energy and direction after collision are derived from the conservation of energy and momentum. Upon collision, the following scattering data are calculated in order to obtain the energy loss and scattering angle in the laboratory system:

$$x^2 = \frac{1}{(A^* + 1)^2} (v_1^2 + A^{*2} V^2 + 2A^* v_1 V \cos a) ,$$

$$v^2 = \frac{A^{*2}}{(A^* + 1)^2} (v_1^2 + V^2 - 2v_1 V \cos a) ,$$

$$\cos C = \frac{1}{x(A^* + 1)} (v_1 + A^* V \cos a) ,$$

$$\cos N = \cos \lambda \cos C \sin \lambda \sin C \cos \phi' ,$$

$$v_2^2 = x^2 + v^2 + 2xv \cos \lambda ,$$

and

$$\cos \psi = \frac{1}{v_2} (v \cos N + x \cos C) .$$

The flight parameters in the above equations are defined as follows:

- $\vec{x}$ - velocity of the center-of-mass of the collision system
- $\vec{v}$ - neutron velocity after collision in the center-of-mass system

- A^* - effective mass of the target atom
- a - angle between $\vec{v}_1$ and $\vec{V}$
- λ - center-of-mass scattering angle
- C - angle between $\vec{x}$ and $\vec{v}_1$
- N - angle between $\vec{v}$ and $\vec{v}_1$
- ψ - laboratory system scattering angle
- ϕ' - azimuthal angle of $\vec{v}$ around $\vec{x}$
- $\vec{v}_2$ - neutron velocity after collision in the laboratory system.

Chemical binding of the target atoms increases the inertia of the target in collision. The influence of chemical binding can be approximated in these calculations by allowing the target atoms to take on a larger mass, A^* , than the true target mass, A . When the thermal motions of the target atoms are being considered, a table giving a value of A^* for each element must be included in the input data.

The polar scattering angle in the center-of-mass system, λ , is selected from an isotropic distribution, and the azimuthal scattering angle, ϕ' , is selected from a distribution uniformly distributed in the interval of 0 to 2π . The azimuthal angle, ϕ , which determines the rotation of the emergent neutron about its previous direction, is also chosen from a uniform distribution in the interval of 0 to 2π . The scattering angle, ψ , and the azimuthal angle, ϕ , are used to determine the direction cosines of the neutron after collision.

When the incident neutron energy is less than ETM, neutron scattering is treated as isotropic in the laboratory system, with no energy loss or gain. The direction cosines, after collision, are chosen, assuming isotropic scattering, by using a rejection technique.

5.3 GAMMA SCATTERING EVENTS

All gammas are forced to undergo collisions that are either a Compton-scattering event or a pair-production event. The type of event is selected by determining if the difference, $\left[\sum J, C(E) / \sum J, S(E) \right] - R$, is positive. If the difference is positive, the collision is assumed to be a Compton-scattering event. If the difference is negative, the collision is assumed to be a pair-production event.

If the event is a Compton-scattering collision, the energy and direction after collision are selected at random from the Klein-Nishina formula by using a rejection technique developed by H. Kahn (Ref. 10). The technique used to select both a random scattering angle, ψ , and a random energy, MeV, after a collision, is illustrated in Figure 5-2. The azimuthal scattering angle, ϕ , is taken to be uniformly distributed in the interval of 0 to 2π . Direction cosines in the fixed reference system are computed by using equations for α' , β' , and γ' , which are given in Subsection 5.2.1.

The selection of the pair-production interaction as the collision event will result in the creation of an electron-positron pair. It is assumed that the annihilation of the electron-positron pair will occur before they have moved any appreciable distance from the collision point. The annihilation of an electron-positron pair results in the production of two isotropically emitted photons, each with an energy of 0.51 MeV. Only one photon with energy of 0.51 MeV is followed in the program, but the weight is doubled to account for the fact that two photons were actually emitted. A rejection technique for isotropic scattering is used in the procedure to compute the direction cosines of the emitted photon.

The weight of the gamma ray after collision is given by

$$W' = W \frac{\sum J, S(E)}{\sum J, T(E)},$$

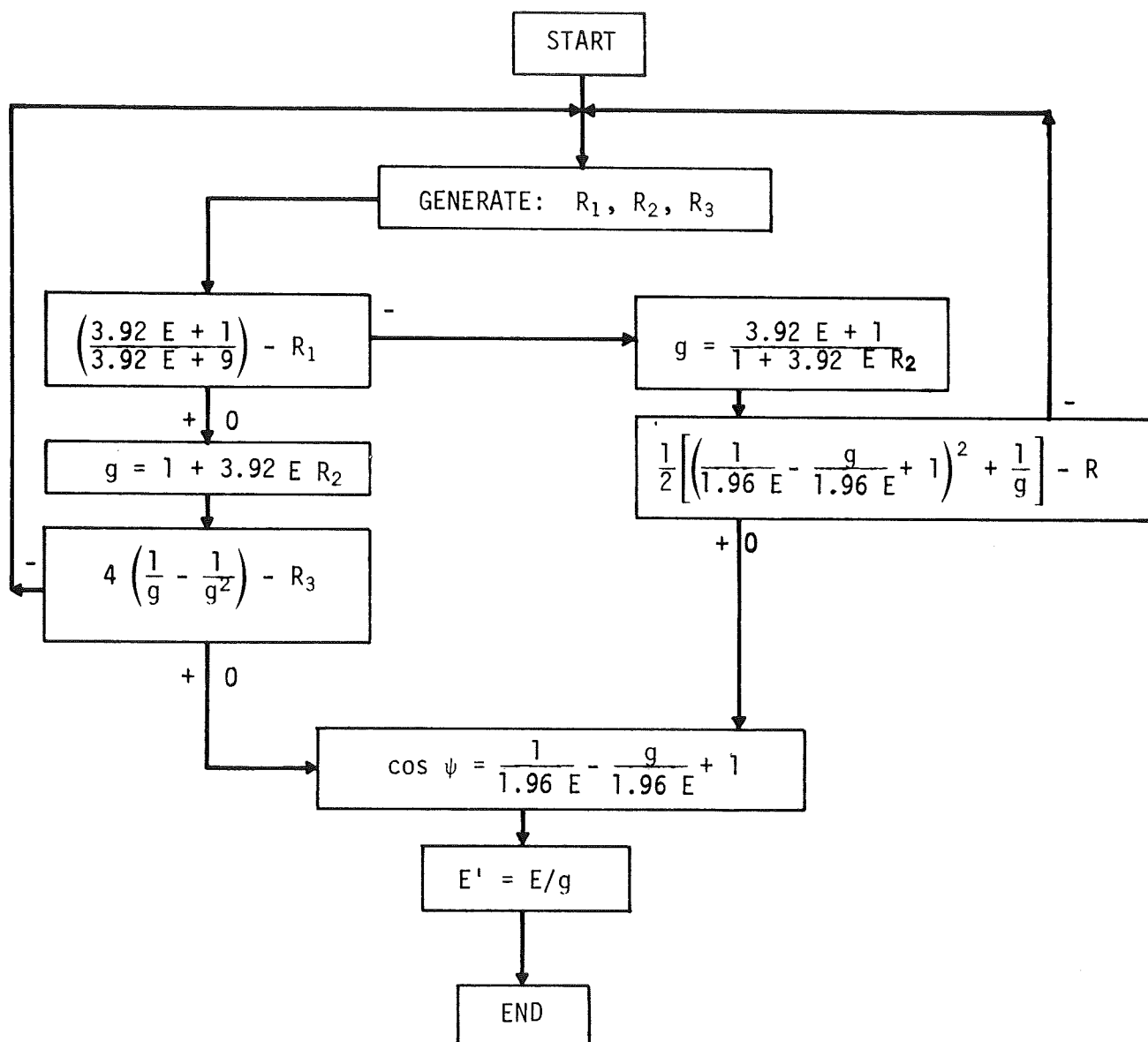


FIGURE 5-2. REJECTION TECHNIQUE FOR SELECTION OF SCATTERING ANGLES AND SCATTERED ENERGIES FOR COMPTON COLLISIONS

where the collision is taken as a Compton-scattering event, and by

$$W' = 2W \frac{\sum_{J, S} (E)}{\sum_{J, T} (E)},$$

when the collision is taken as a pair-production event.

5.4 ENERGY DEPOSITION

The H01 routine of CAVEAT computed the energy deposition caused by scattering, absorption, and termination for each geometric region. This energy, plus a standard deviation value, is included in output of the H01 routine.

The energy deposition at each collision is computed whenever the incident particle energy, E , is greater than an input parameter, ELD. When E is less than ELD, no energy deposition is computed. The energy deposition from an absorption in region J containing the collision point is computed as

$$ED_1 = W \frac{\left[\sum_{J, T} (E) - \sum_{J, S} (E) \right]}{\sum_{J, T} (E)} E,$$

where

- W - particle weight before collision
- $\sum_{J, T} (E) - \sum_{J, S} (E)$ - macroscopic absorption cross section for J th region at energy, E (photo-electric events for gammas)
- $\sum_{J, T} (E)$ - macroscopic total cross section for the J th region at energy, E
- E - particle energy before collision.

The energy deposition from particle scattering is given by

$$ED = W \frac{\sum_{J, S} (E)}{\sum_{J, T} (E)} (E - E' - ET) ,$$

where E' is the energy after the collision. The parameter, ET , depends upon the type of particles (neutrons or gammas) and also on the type of scattering event. For neutrons, ET is E_x , the excitation energy. Hence, the energy, $E - E' - E_x$, is the neutron energy given up as kinetic energy to the collision nucleus. The excitation energy is given off in the form of inelastic secondary gammas, and the energy deposition resulting from collisions by these gammas is treated as a separate problem. For elastic scattering, E_x is zero. For gamma collisions, ET has a value of 0.51 MeV for pair-production events and zero for Compton-scattering events.

5.5 TIME OF FLIGHT CALCULATIONS

The addition of the time dependence to the CAVEAT code required the calculation of the time necessary for particles to travel from a source or collision point to the next collision or detector point. These straightforward calculations are performed at every collision, and a running sum is kept on each particle to obtain its age. For neutrons, the time, T , depends only on the energy of the neutron, E , and the distance traveled, S , :

$$T = (7.23 \times 10^{-10} * S) / \sqrt{E} ,$$

where the energy is always converted to MeV units. Relativistic effects on the neutron have been neglected, (~ 1.1 percent error at 14 MeV). For gammas, only the distance traveled, S , is needed, since gammas move at the speed of light:

$$T = S / (2.99776 \times 10^{10})$$

5.6 PARTICLE TRACKING TERMINATIONS

Since the tracking, or history technique, used by CAVEAT does not allow for an absorption to occur, but only allows scattering events, a particle will never "die". To terminate the tracking of a given particle, one of the following events must occur:

- The particle's energy is reduced below the minimum energy, EMIN.
- The number of collisions with any energy supergroup exceeds the maximum allowable, MAXCOL.
- The particle's age exceeds the maximum age limit, TMAX.
- The particle has a collision at a distance, D, from the origin of the coordinate system, so that $D \geq DMAX$.
- The particle escapes into the outside region, Region 2.
- The particle's weight is reduced below the minimum weight, WMIN.

The quantities, EMIN, MAXCOL, WMIN, DMAX, and TMAX, are problem input parameters. Whenever the particle weight drops below WMIN, Russian Roulette is played to determine whether the history is to be terminated or continued. The Russian Roulette parameter, RR, is compared with a random number, R. If $RR \geq R$, the history is continued with a new particle weight, $W' = W/RR$. If $RR < R$, the history is terminated.

6. ANALYSIS ROUTINES

The CAVEAT code has two routines, A01 and A02, that analyze the collision data generated by the H01 routine. The A01 routine estimates the fluence, or flux, at point detectors. (Throughout this section, the quantity calculated by A01 will be called a fluence, even though for some problems this quantity may be flux or some other quantity of interest in radiation transport.) Both the scattered and unscattered (virgin) fluence is estimated, being recorded as a function of energy, time, polar angle, and azimuthal angle at the specified detector points. The A02 routine gives an estimate of the average track length within each geometric region, which can be converted to flux by dividing by the volume of the region. The track lengths are recorded as a function of region and energy. In addition, the angular distribution of the current leaking into the outside region, Region 2, and a leakage particle source file can be obtained from A02.

6.1 A01 ANALYSIS ROUTINE

The purpose of the A01 analysis routine is to estimate the fluence at a set of point detectors. The collision data required by A01 for each collision is

- Spatial coordinate of collision and source points
- Direction before collision
- Energy before collision, or at source
- Weight after collision, or at source
- Age at the collision, or at source
- Type of collision
- Target nucleus
- Collision or source region.

The scattered fluence estimate is made by summing the value of f in the following expression over all collision points:

$$f = W P_r \left[\frac{\exp(-\lambda)}{d_i^2} \right] ,$$

where

W - weight of the particle after collision

P_r - probability of the particle being scattered through the angle between the direction before collision and the direction from the collision point to the detector.

λ - number of mean free paths from the collision point to the detector

d_i - distance between collision point and detector.

The unscattered fluence is calculated by the above estimator; however, only source points are summed, and P_r is set equal to $1/4\pi$. The procedure for calculating f is given below.

Let the spatial coordinates of a point detector be denoted by x_i , y_i , and z_i , and the coordinates of a collision or source point by X , Y , and Z . The distance between the collision, or source, point and the i th detector point is given by

$$d_i = [(X - x_i)^2 + (Y - y_i)^2 + (Z - z_i)^2]^{\frac{1}{2}} ,$$

and the direction cosines of the flight path to the detector are given by

$$\alpha_i = \frac{x_i - X}{d_i} ,$$

$$\beta_i = \frac{y_i - Y}{d_i} ,$$

and

$$\gamma_i = \frac{z_i - Z}{d_i} .$$

The laboratory system scattering angle through which the particle must scatter in order to be heading toward the detector is computed by the equation

$$\cos \psi_i = \alpha\alpha_i + \beta\beta_i + \gamma\gamma_i ,$$

where α , β , and γ are the direction cosines of the particle before collision. The distances traveled through each region along the flight path, between the collision, or source, point and the detector point, are computed and multiplied by the total macroscopic cross section for the energy after collision for each region to give the path length in each region.

The method used to compute the particle energy after scattering through the angle, ψ , is dependent on the type of particle being considered. If the particle is a neutron, the energy after a collision with any element of atomic weight ratio A (except hydrogen) is computed by using the equation

$$E_i = E \left[1 - \frac{2A}{(A+1)^2} + \frac{A^2}{(A+1)^2} (1-B) + \frac{2A}{(A+1)^2} B^{\frac{1}{2}} \cos \lambda_i \right],$$

where λ_i , the center-of-mass scattering angle, is given by

$$\cos \lambda_i = \frac{\cos^2 \psi_i - 1 + \cos \psi_i (\cos^2 \psi_i + A^2 B - 1)^{\frac{1}{2}}}{AB^{\frac{1}{2}}} .$$

In the above equation, B is a parameter taking on the value $B = 1$ if the collision is an elastic scattering event, and the value

The track length through Region K, when the material in the region is a vacuum, is

$$TL_K = W' S$$

The average fluence for a region is proportional to the sum of the average track lengths in the region for all particles that have a nonzero probability of reaching the region.

The average track length per unit source strength in each region is obtained by dividing the sum of the track lengths in the region by the number of source particle histories from which the collision file was generated.

The average fluence per unit source strength for a region can be obtained by dividing the average track length per unit source strength in the region by the volume of the region. The quantity computed by A02 is the average track length per unit source strength for each region. This quantity is printed as a function of the energy groups defined for that purpose in the A02 input.

6.2.2 Particle Leakage

The weight of a particle entering Region 2, after undergoing a collision in an inside region, is defined by

$$W \ell = W \exp^{(-EXP)},$$

where

EXP - the sum of the mean free paths traveled by the particle between the collision point and the boundary of Region 2

W - the particle weight following the collision

$W \ell$ - an estimator of the number current leaking out of the inside regions.

The sum of the quantities, $W \ell$, computed from each collision is normalized by dividing by the total number of source particles followed. When the input parameter, $LSO = 1$, the normalized number current leaking out into the Region 2 is printed as a function of energy, E , after collision, and the angles, $\cos^{-1} \gamma$. The results so obtained can be used as the energy and angular distribution of a point source representation of the system. When $LSO = 2$, a tape is prepared that contains, for each collision, the following quantities:

- $W \ell$ - normalized number current
- NR1 - number of region from which the particle entered Region 2
- X, Y, Z - coordinates of the entrance point into Region 2
- α, β, γ - direction cosines of the particle
- E - energy of the particle as it enters Region 2
- T - age (set equal to zero).

When $LSO = 0$, no leakage data are computed.

Because each collision generates a leakage particle, the leakage source file may contain more particles than there is computer time available to transport them. To reduce the number of leakage source particles, two termination parameters were added to the CAVEAT code. The first parameter, ELOCUT, prevents any leakage particle with energy less than ELOCUT from being written on the leakage file. The second parameter, WLOCUT, along with the Russian Roulette parameter, RR, terminates leakage particles with weights less than WLOCUT, unless these particles successfully play Russian Roulette. The weight of particles that are successful is increased by dividing it by RR.

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