TID/SNA--270

To AEC-NASA Space Nuclear Systems Office

SRT-FRS20-W393a1

FINAL REPORT -- CY-1970

SHIELDING CODE IMPROVEMENTS

PROJECT 393, CONTRACT SNP-1

NERVA Program, Contract SNP-1

February 1971

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February 1971

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ABSTRACT

This report describes work performed under Project 393 in the SNP-1 contract for Contract Year 1970. This project covers work in the development of improved shielding and radiation analysis computer codes.

Work was carried out in three general areas:

- 1) Code Coupling Improvements
- 2) Biasing in Monte Carlo Calculations
- 3) Monte Carlo Code Improvements

Each was an extension of CY-1969 efforts to provide ANSC and NERVA with an efficient system of computer codes for analysis of difficult radiation transport and shielding problems. Efforts in CY-1969 were directed primarily toward producing the basic methods for solving these problems. Work in CY-1970 was directed mainly toward giving these methods the flexibility and efficiency for precise and economical analysis of the problems. Comparisons have shown that the techniques give results comparable with those by other methods and, in most cases, at a fraction of the cost.

ACKNOWLEDGEMENT

Under subcontract, Radiation Research Associates (RRA), Fort Worth, Texas, assisted in the modifications of the COHORT Monte Carlo code and performed the biasing studies reported here.

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I. INTRODUCTION AND SUMMARY

During the past two years, nuclear analysis in the NERVA development program has significantly increased in level of detail. Prior to this time, most analyses were approximate parameter studies. Many present analyses, on the other hand, provide detailed descriptions of radiation environment as needed for engine and component design. In accomplishing this greater detail, the general tendency is for greatly increased cost for these analyses due to increased computer time. The general technique used to accomplish this improved detail is the use of the Monte Carlo method. Computer codes which use the Monte Carlo method simulate individual particles of radiation and calculate the general environment by summing a large number of these individual particles. Other methods have inherent limitations in that they attempt to predict the environment without considering all of the information which determine it. In some limited analyses, this more approximate approach is sufficient, but can only be used as special cases and must be supplemented by Monte Carlo to meet the design requirements for an entire system.

In meeting these requirements, an approach which could be used is to calculate everything by Monte Carlo. This would provide the necessary information but could be prohibitively expensive in computer time. Economies can be found in using the Monte Carlo codes by considering the needs of the particular analyses. Further economies can be found by using supplementary methods when the results would be adequate for the information requirements. A modest program of methods development under SRT funding has provided, for the past two years, the means for accomplishing the detailed analyses of the Monte Carlo method while employing a number of techniques for limiting their cost.

A. Code Coupling Development

In many analyses Monte Carlo may be necessary for part of the analysis, but is not necessary for another part. Methods have been developed for using less expensive methods, where possible, in concert with the Monte Carlo method. Frequently, the discrete ordinates method can be used for detailed calculations but must be supplemented with Monte Carlo for an entire analysis. In CY-1969⁽⁵⁾ an original code was written which provides the data transfer link between the two methods. This code, DASH, was used for several analyses in CY-1969 and CY-1970 and is presently being used in a large fraction of the analyses performed for NERVA. In CY-1970, DASH was revised several times to provide coupling capability with additional codes and to provide specialized data for several purposes. In addition, coupling development was carried out in using data internal to the discrete ordinates code, DOT, and in processing the tapes used to link the codes.

B. Biasing Studies

In using the Monte Carlo method to simulate the paths of individual particles, the nearest mathematical analogy to the physical case is seldom used. Those particles which contribute least to the final result are treated only approximately and those which contribute most are given the best analogy. In this way, unnecessary computer time is avoided. The technique is called biasing. The choice of which to treat approximately is primarily a matter of judgement and a conservative choice is usually made in order to be certain of the answer. A preliminary study was made in CY-69 to determine if information from a mathematical optimization could be used to choose the best biasing. On the basis of this study, additional work was done in CY-1970 to determine which biasing techniques available in FMC and COHORT show the greater promise for reducing computer time. Modifications were made in COHORT to use approximations to the

mathematical optimum condition to determine the biasing parameters for gamma ray calculations.

C. Monte Carlo Development

In CY-1969, the COHORT Monte Carlo code package was obtained and made operable on the AGC computer system. Codes were written to provide data from the ENDF/B standard cross-section library for the COHORT and FMC Monte Carlo codes. A common geometry description routine was included in FMC and the point kernel codes. In CY-1970, this description was extended to COHORT. Further modifications to COHORT in CY-1970 provided the capacity to calculate unscattered radiation environment, previously a limitation in the COHORT package. COHORT was also modified to provide a restart tape capability for linking data from different COHORT analysis to minimize duplication of calculations. Additions were made to the COHORT package to provide an estimation of the statistical uncertainty of calculated values.

D. Summary of CY-1970 Accomplishments

Computer code improvements in CY-1970 have extended the techniques developed in CY-1969 to provide an efficient system for nuclear analysis of complex systems. The techniques can now offer a new level of simultaneous precision and economy of calculation. For problems involving both densely and sparsely distributed materials, the techniques reduce the cost of detailed analyses to a fraction of the previous cost.

A system of computer codes has been developed which allows the best aspects of the discrete ordinates and Monte Carlo methods to be used. In this way, many of the limitations of either method are avoided, reducing the cost of analyses. Complete flexibility is possible in the degree to which one method or the other can be employed for any suitable problem.

The codes have been revised to provide a maximum commonality of description and allow a smooth transfer of data from one to another. Other codes have been written to provide interfaces between codes which handle radiation transport data by different methods. Further revisions have provided the means for viewing details necessary for carefully analyzing the origins and causes of calculated radiation environments. This flexibility has been developed primarily through additions to the coupling code DASH* and the COHORT** Monte Carlo package of codes.

In the radiation transport analysis of a system as complex as that of the NERVA engine, there can be no single analysis that will provide all important information. Such an analysis would be prohibitively costly, providing more information than is needed for many parts of the analysis in order to provide sufficient information for another part. Each analysis must be tailored to suit its information needs so that it is done as efficiently as possible while providing the required accuracy. The techniques which have been developed under this project provide sufficient flexibility within the most sophisticated methods available to meet this requirement.

*An original code, written by Aerojet Nuclear Analysis personnel in CY-1969 under Project 393. See glossary of terms.

**A collection of related codes added to the Aerojet library in CY-1969 under Project 393. See glossary of terms.

II. Code Coupling Development

A. Energy Interface Bridging

In calculating radiation transport using Monte Carlo, there may be local regions where neutron thermalization is important. Since thermal neutron transport by Monte Carlo may not be sufficiently accurate without expending considerable computational effort, an energy interface bridging was developed. Thermalization would be calculated by an S_N code (DOT-II was used) based on input information from a Monte Carlo neutron calculation (COHORT was used).

The procedure followed was to create a thermal neutron source using Monte Carlo particle information in the region of interest. This would then be used by the DOT program to calculate the transport and distribution of thermal neutrons.

The first approach was to create a boundary source tape from the particle information. This proved to be unworkable because of ambiguities in defining the proper boundary to which a given particle contributes. As an alternative approach, the COHORT history routine, H01, was modified to save data on tape for all particles whose energies had been degraded below a thermal cutoff. An auxiliary code, PARBIN, was written to use this data to provide isotropic first collision volume sources for DOT. Since the method would be used only where there is significant thermalization, and thus many collisions, the assumption of isotropy at the first collision below thermal cutoff is not unreasonable. It is expected that the most severe limitation of the method is the two-dimensional requirement of the DOT code.

B. Internal Coupling

The DASH coupling code is designed to produce Monte Carlo data from surface angular fluxes calculated by the DOT S_N code. For some applications it is useful to operate on angular flux data at interior regions. This data is available on a tape produced by DOT. A processing code, MONDRIAN, was written to use this tape. MONDRIAN is able to perform two coupling functions: (1) produce internal boundary coupling data for DASH, and (2) produce restart data for DOT.

In the first case, MONDRIAN searches all angular flux data and collects those at prescribed axial or radial internal surfaces. These data are saved on tape in a format used by DASH. This allows DOT-DASH coupling, through MONDRIAN, at any axial or radial surface of a cylinder analyzed by DOT. This has found immediate useful application in producing Monte Carlo source data for the COHORT code at surfaces within an original S_N DOT problem. In this way the Monte Carlo method was used to calculate greater angular detail in the outer regions than is possible in the S_N format.

In the second case, MONDRIAN can be used to provide restart data for DOT. After a slight modification, DOT has been made to accept scalar flux and angular moment data from other DOT problems as first guesses for a second DOT problem. This can potentially save computation time in the second DOT problem. MONDRIAN produces this data (also available on the scalar flux tape) from the angular flux tape and saves it on a second tape in the format required for DOT restart. This technique has found use in restarting a partially converged problem, rerunning a DOT problem with material density changes from the first problem, or rerunning with a different order of angular expansion.

C. Additions to the DASH Code

Several modifications have been made in the DASH code during CY-1970 to broaden its capabilities. In addition to extending the coupling technique to other codes, several changes were made to improve the efficiency and flexibility of the code. A general flow chart of the coupling capacity developed through the end of CY-1970 is shown in Figure 1. A short discussion of each of the CY-1970 modifications to DASH follows.

1. FMC to DASH Coupling - In CY-1969 DASH was programmed to produce particle data suitable for use as a source for the Monte Carlo codes FMC and COHORT. In CY-1970 the code was modified to allow the same FMC format data to be used for source data for DASH. (See Figure 1). In this way a restart of DASH is possible, bypassing the sampling procedure. This data can then be used to calculate further transport or changed to provide source data for another code. Alternatively, data produced by FMC itself can be used by DASH if ordered by descending particle energy to simulate the energy grouping used in S_N . A sort procedure has been devised whereby the necessary ordering is accomplished.

2. DASH to FASTER Coupling - - Modifications have been added to the DASH code which produce source data for the FASTER Monte Carlo code. FASTER is a highly biased Monte Carlo code which has the potential for doing very rapid calculations. Some difficulty has been experienced in interpreting results due to the biased nature of the code, so it may be limited in usefulness for absolute results.

FASTER requires data in a probability distribution format. DASH modifications allow the production of source data cards by running a series of stacked DASH cases, one case for each source. By using a series of normalizations, the probability tables generated for FASTER sources

Figure 1 - DASH Coupling Information Flow

reproduce the S_N angular fluxes exactly for the most significant directions. Several of these primary probability tables are usually averaged, however, to produce a single source to facilitate economy. Further detail using FASTER is not recommended, however, as the code probably should not be used to replace other more precise Monte Carlo codes, such as COHORT, MORSE, or FMC.

3. Control Routine for Flexible Dimensioning --

The DASH code may require up to 400,000 bytes of core storage on an IBM 360. The addition of overlay structure reduces this by about 20 per cent by reusing some storage locations when they are no longer needed for their original purpose.

Since variable arrays must be dimensioned (thus allocating storage) to allow for the largest number of possible values of the variables, in many cases much of the storage is not used. To avoid leaving unused storage, a control routine was written for DASH which allocates only that storage needed for a particular case. Using the control variables from the card input, this routine calculates the array sizes for dimensioned variables and stores in COMMON the location of the first value of each variable. While this method saves an additional 25% of storage for most cases, it increases the computer time by about 40% so is not particularly useful where sufficient core storage is available. An effort has been made to preserve two versions of DASH, one with and one without this flexible dimensioning feature.

4. General Detector Orientation --

Changes were made in the DASH code such that detector surfaces can be designated under one of three options: upward, downward, and general. Under the first option, upward, particles are sampled from DOT angular fluxes in an upward direction and traced to radial intervals on a plane perpendicular to the polar axis. Under the second option, downward, particles are sampled from DOT angular fluxes in a downward direction and traced to radial intervals on a plane perpendicular to the polar axis. The third option, the one developed under this task, allows for both upward and downward directed particles.

The detector surfaces are specified by pairs of (r, Z) coordinates so that the detectors can be any linear surface. The upward and downward options require detectors to lie on planes with constant Z .

5. Fit Parameter Flexibility - - In CY-1969 DASH was programmed to provide a choice in methods for assigning particle weights to individual sample vectors. An option allowed particle weight assignment to correspond to S_N tabular values or to be interpolated from S_N values. The interpolation was implemented by least-squares fitting to flux variation in the two angular and one spatial parameters available from S_N .

In CY-1970 the options were extended to provide much greater flexibility in the means of fitting these data. One option allowed the fitting to be accomplished in the two angular parameters only, using non-interpolated (histogram) values in the spatial variable. Two more options were added when some least-squares fits in the polar angle failed to properly represent an interpolation smoothing of the data. The first of these two options was to test for the particular failure observed and substitute a histogram (corresponding to S_N tabular values) in angles for those spatial intervals where it occurred. The second option was to do the polar angle fitting by a least-squares fit to the logarithm of the polar angle, thus avoiding the difficulty. This final option has proven to be the more useful to date in problems involving leakage from the NERVA pressure vessel and reactor assembly (PVARA).

6. Leakage Interval Specification - - To better understand the origins of radiation external to the PVARA, DASH was modified to choose particular spatial intervals. With this option and other sampling options already provided, DASH is now able to look at any sequence of intervals on the side and any sequence of intervals on either end in a single case or separate cases.

7. Normalization -- An option was added to provide for spatial and energy dependent normalization of all data handled by DASH. The normalization factor can be multiplied at the source interval and/or at the detector. This technique has been used as a first approximation to the effect of changes in design of the PVARA to meet certain external radiation level criteria and to apply uncertainty factors.

8. Rotation for Gimbaling -- Modifications were made in the DASH code to allow coordinate rotation in the particle descriptions for coupling to Monte Carlo codes. In this way it is possible to describe particles for Monte Carlo as if they had come from a source rotated from its real position. This was used to provide Monte Carlo data to analyze the effect of gimbal rotation of the NERVA engine on radiation above the propellant tank.

9. Asymmetric Quadratures -- The quadrature description subroutine, IGLOO, was modified to accept general quadrature descriptions. The earlier version depended on symmetry in the two direction cosines to complete the description. The present version allows the use of asymmetric quadrature sets that have been tailored to provide detail in any direction of interest. No provision for interpolative fitting of asymmetric quadrature information was made since the two techniques are designed to accomplish the same purpose. There is no need to interpolate asymmetric quadrature data since such sets are normally designed to produce the desired degree of detail that the interpolative techniques attempt to construct from low order data. No FASTER source data can be produced directly from results obtained from asymmetric quadrature calculations.

10. Submission to Code Centers -- The DASH code, as it existed in May, 1970, was submitted to the Radiation Shielding Information Center, Oak Ridge, Tennessee, and the Computer Software Management and Information Center, Athens, Georgia. The version submitted included the control routine for flexible dimensioning and general detector orientation modifications from the CY-1970 tasks.

The information submitted to the centers included a tape containing the code and a sample problem plus a copy of SRT-TRM01-W393-4C "Technical Report and User's Manual, DASH - FORTRAN IV Void Tracing and S_N - Monte Carlo Bridging Code". At the same time the code was approved for announcement as a NASA technical brief.

D. Multiple Source Techniques for Coupling

A short code was written to sum and convert formats of particle tapes used for Monte Carlo source data. This code, ADD, uses one to three input tapes in any combination of FMC and COHORT formats. Using this data it can produce a single tape of Monte Carlo data in either the COHORT or FMC format. If the FMC format is produced, the tape can be sorted so that the particles will be in the order of decreasing energy as required by DASH for multigroup handling.

DASH can provide data format conversions from DOT or FMC to DOT, FMC, COHORT, or FASTER. Two other short codes were written to further expand the format flexibility. The code FMCPD can produce cumulative probability tables from FMC data and the code SOTAG can produce FMC data from these tables.

Using the codes ADD, DASH, FMCPD, SOTAG, and MONDRIAN it is possible to handle any number of pieces of source data in CPD tables, DOT leakage angular fluxes, DOT internal angular fluxes, COHORT particle data, or FMC particle data. These data can then be converted for use in parts or in total by DOT, FMC, COHORT, or FASTER within the inherent limitations of each code.

III. BIASING STUDIES

These studies were investigations of biasing techniques in Monte Carlo. This includes a study to determine which of the biasing options available in FMC and COHORT were best suited for use in NERVA shielding studies and the optimum biasing parameters to be used with each method. In this study, a code designated BIPAR was written to calculate the exponential transformation parameters needed for input to COHORT and FMC from a knowledge of the adjoint flux for a one dimension mock-up of the problem.

As a continuation of the investigation started in the previous year, a method was developed for implementation into COHORT which would permit importance sampling to be used in determining scattering angles and track lengths within a random walk. The method which was developed for COHORT is limited to gamma ray transport. In developing the method, it was assumed that the importance function would be specified by the adjoint function.

While theoretically attractive, insufficient experience has been gained with these techniques to fully evaluate their usefulness. A detailed discussion of these studies is attached as an appendix.

IV. MONTE CARLO DEVELOPMENT

The COHORT Monte Carlo procedure has been used extensively for radiation shielding and environment studies on NERVA. The results of these studies have indicated that desirable improvements should be made to COHORT which would increase the capabilities and economy of the code in future NERVA studies. Improvements in three different areas have been incorporated into the COHORT procedure. The improvements include:

1) modification to include an expanded geometry capability that has a geometry specification format compatible with that required by FMC, FASTER GGG, and QAD, 2) the development of routines to calculate the direct beam component for anisotropic and distributed sources, 3) provisions to generate restart tapes to allow COHORT-COHORT and COHORT-DASH coupling, and 4) modifications to allow the calculation of standard deviations in COHORT.

A. FASTER Geometry Format

One of the most time consuming task in running radiation transport codes such as COHORT, FMC, and QAD is that of describing the configuration involved with a mathematical model. The mathematical model must be described in the specified format for each code to be used. Much of the set up time required to prepare the input data decks can be saved if all codes used in the NERVA shielding studies have a common geometry specification format. Both the FMC and QAD procedures have been previously modified at ANSC to include the FASTER geometry subroutines. The H01, A01, A02, and A03 routines of the COHORT procedure were modified to include the FASTER geometry routines.

In addition to providing a common geometry format for each of the transport codes, the FASTER geometry routine also provides additional geometry capabilities as well as various time saving features. These features include:

- 1) Provisions for describing volumes of revolution about each of the 3 axes (i.e., X-, Y-, Z- axes).
- 2) Provisions for using the general quadric equation to describe boundaries.
- 3) Eliminates the need to define in the program input a most probable region for each boundary used to describe each region.

- 4) Eliminates the need to define in the program input the number of boundaries used to define each region.
- 5) Eliminates the need for hand checking the mathematical model for reflected regions and holes. The FASTER geometry subroutine performs the necessary consistency checks internally.

Thus, the modifications to include the FASTER geometry subroutines in COHORT not only provide an extended geometry capability but, also saves setup time by 1) requiring only one geometry description per configuration, 2) reducing the required input, and 3) eliminating the need for hand checking of the mathematical model.

B. Direct Beam Capability

1. AO3 Analysis Routine

The AO1 analysis routine of COHORT calculates the scattered flux component to a point detector. If the radiation source is such that the source has an isotropic angular distribution, then the routine will also calculate the direct beam flux component as well as the total flux. However, if the source is anisotropic, such as the PVARA source (pressure vessel and reactor assembly) in a typical NERVA configuration, then the direct beam component cannot be calculated properly with the AO1 routine. In previous NERVA studies, to determine the direct beam component it was necessary to define a simplified mathematical model and use a routine such as DASH to do the calculations. This required additional time to describe the model and prepare the DASH input. To eliminate these problems a new routine for COHORT, designated AO3, was developed.

The AO3 routine is designed to read source particle parameters (i.e., spatial position, direction, energy and weight) from a "source" tape. The source tape input to AO3 must contain particle parameters for each source

particle that are in the same format as source tapes produced by the SOL routine. The path of each source particle through the defined geometry is determined from the particle parameters by projecting the path from the source point in the specified direction until it reaches an outer boundary of the defined geometry. The length of the particles' path through each geometric region intersected is recorded as a function of region.

The weight of the source particle is denoted by W . The probability that the particle will undergo a collision within the distance S through the region J which contains the source point is defined as

$$[1 - e^{-S\Sigma_{J,T}(E)}], \quad (2.1)$$

where $\Sigma_{J,T}(E)$ is the total macroscopic cross section for region J at the energy E of the particle.

The particle expectation track length through region J for the particle is given by

$$TL_J = \frac{W}{\Sigma_{J,T}(E)} (1 - e^{-S\Sigma_{J,T}(E)}). \quad (2.2)$$

The weight of a particle entering region number K , a region not containing the source point, is

$$W' = W e^{-EXP}. \quad (2.3)$$

where EXP is the sum of the mean-free-paths traveled by the particle along the flight path before intersecting a boundary of region K . The average expectation track length through region K is

$$TL_K = \frac{W'}{\Sigma_{K,T}(E)} (1 - e^{-S\Sigma_{K,T}(E)}). \quad (2.4)$$

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

$$TL_K = W'S. \quad (2.5)$$

The expectation flux for a region is proportional to the sum of the average expectation track lengths in the region for all particles that have a non-zero probability of reaching the region.

The average expectation 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 particles.

The expectation flux per unit source strength for a region can be obtained by dividing the average expectation track length per unit source strength in the region by the volume of the region. The quantity computed by program A03 is the average expectation 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 program input.

Results may be obtained from any source that has been defined on tape in a format comparable to that produced by the S01 routine. Specifically, the source tape generated by DASH may be used as direct input into A03.

2. Modification of A02 Analysis Routine

From the code coupling point of view; e.g., using a source tape from DASH, H01 or A03 can use anisotropic data directly. The H01 routine can be used to produce the HIST1 tape of collision data. This can be used as source information with A01 to calculate scattered radiation at point detectors. Alternatively, a source tape from DASH can be used with A03 to calculate direct radiation at volume detectors. The A02 analysis code uses HIST1 collision data from H01 as a source also. Since HIST1 contains the original

source data from DASH as well as the collision data, it can be used to calculate total (direct plus scattered) radiation to volume detectors. Modifications have been made in A02 to separate out the contribution to the total by the original DASH data included on HIST1, thus including the results of A03 as part of the normal H01/A02 procedure.

With this additional modification it is now unnecessary to run A03 to obtain the direct component of radiation if the total radiation is desired as calculated by A02.

C. COHORT Restart Capability

In the proposed NERVA systems, the configurations are very complex and contain large regions of high density as well as low density materials. Also, a number of the configurations being studied are very similar with the exception of a small section such as the payload. With this in mind, it was determined as a result of previous radiation analyses that future calculation could best be performed by:

- 1) Not using a single method of radiation transport such as Monte Carlo or S_N discrete ordinate. Instead, both methods should be used for the transport of the particles in the part of the configuration for which it is most applicable. For example, the Monte Carlo method should be used for the radiation transport in the parts of the configuration that require a 3-dimensional geometry or consist of a large region of low density material.

- 2) Not repeating the transport calculations for that part of the configuration that remained unchanged.

To perform the transport calculations according to these criteria, the necessary information must be transferred between successive calculations. If this transfer of data is done external to the codes involved, much time consuming hand data preparation is required. The chance for data handling errors is also introduced. Thus, a means of coupling the successive calculations is very desirable. The desired coupling may be Monte Carlo-Monte Carlo or Monte Carlo- S_n . The necessary modifications have been made to COHORT to provide internal coupling (i.e., no external data handling) in the form of restart tapes between COHORT-COHORT and COHORT-DASH.* The restart tape is a magnetic tape that contains the necessary data for input into a successive calculation. The DASH procedure is designed to generate restart tapes in the proper format for input into the S_n code DOT or FMC.

In the H01 routine when a particle history terminates due to a particle escaping the attenuation media into an outside, unbounded region, a check is made to determine if the leakage parameters are to be saved on a restart tape. If a restart tape is to be generated and the region into which the particle escapes is specified as one for which entering leakage particles are to be described on the tape, the location of the outside boundary intersection and the direction cosines, energy, and weight of the particle are written on the tape. This tape is in the correct format for input in a successive H01 calculation as a source tape or for input into DASH* which in turn will generate a source tape in the proper format for input into DOT or FMC.

*DASH cannot accept COHORT format directly but requires an intermediate handling by the ADD code to produce an equivalent tape in the FMC source format.

D. Calculation of Standard Deviation

In the standard COHORT package, no provision has been made for estimation of the statistical accuracy of results. In order to provide this capability, the analysis routines A01, A02, and A03 have been modified to calculate the standard deviations of the results. This, in general, is calculated by equation (2-6), below.

$$S = \frac{1}{\sqrt{N-1}} \left\{ \frac{1}{N} \sum_{i=1}^N X_i^2 - \frac{1}{N^2} \left(\sum_{i=1}^N X_i \right)^2 \right\}^{\frac{1}{2}} \quad (2-6)$$

where

S = Standard Deviation

N = Number of Histories

X_i = Result of the i th History

If the total result of all histories is

$$X = \sum_{i=1}^N X_i / N \quad (2-7)$$

then it can be said that there is approximately a 68% probability that the "right" answer lies between $X + S$ and $X - S$. Similarly, there is approximately a 95% probability that the "right" answer lies between $X + 2S$ and $X - 2S$. This analysis, of course, does not account for errors resulting from:

1. Incorrect Monte Carlo model
2. Incorrect source description
3. Uncertainties in cross sections.

The entire COHORT package, as operable at Aerojet Nuclear Systems Company, is shown schematically as Figure 2. In addition to the improvements mentioned above, Figure 2 shows the response function and secondary gamma source modifications to A02.

FIGURE 2
AEROJET COHORT MONTE CARLO PACKAGE

V. COMPARISON OF COUPLING TECHNIQUES IN A NERVA RADIATION ANALYSIS

Many of the techniques developed in CY-1969 and CY-1970 were used in an analysis of the NERVA system conducted to evaluate calculational methods. This analysis used DOT for analysis of the PVARA and COHORT outside the PVARA. Different quadrature orders were used in DOT and different coupling interfaces used to ascertain the limitations of the method.

In sampling DOT results in DASH, it was necessary to devise a means of simulating physical particles from S_N information. The S_N fluxes are tabulated in energy, space, and angle. One could define a "particle" for each combination in terms of the particles/second value of the tabulated flux. These vectors, if continued by Monte Carlo through a void or low density region, would not necessarily intersect regions of interest. This is comparable to the "ray effects"⁽¹⁾ obtained if the S_N model contains voids. To more nearly represent the physical problem, the particle directions must be distributed uniformly over that part of the igloo that can be seen from the regions of interest.

Histogram

The easiest way that particles can be produced to emerge between the vectors predicted by S_N is to sample a uniform distribution of vectors and assign to each vector that emerges through any block its share of the particles/sec value of the S_N vector in that block. This is equivalent to a histogram in angle with constant particle current within the solid angle intercepting the block. Tracing the particles evaluated in this mode results in a spatially oscillating flux at a distant surface. In particular, radiation coming from the end of the PVARA will generally be underpredicted near the polar axis and radiation from the side will be overpredicted directly above the outer radius of the reactor.

Smoothing

In order to improve on the histogram results, a system of least-square curve fits in polar and azimuthal angle was devised. This results in a smoothly varying assignment of particles/sec to vectors at all angles and produces a smoothly varying flux at distant surfaces. The values at the polar axis and above the reactor radius, in general, are improved by the smoothing procedure but are limited by the extrapolation of the curve fits from the nearest S_N vector.

Tailored Quadratures

The quadrature set, that set of angles defining the S_N vectors, can be tailored to a particular analysis to remove the need for extrapolating curve fits over angles of several degrees. This can improve the accuracy by providing that several of the "blocks" of a more refined igloo can be seen from the detector surface.

Comparison of Methods

A computer program was written to accept surface angular flux data from the S_N code, DOT⁽²⁾ and produce the necessary fitting and sampling. This code, DASH^(3, 4) can also calculate the transport of the sampled vectors through a void or pure absorber.

As an example of the results from histogram, smoothed, and tailored quadrature modes, a series of calculations was performed using an S_6 quadrature set and an S_{124} quadrature set.* The results from the S_6 calculation were treated in the histogram mode and the smoothing mode. Since the S_{124} results were tailored to use very small steps in angle in the direction of interest, only the histogram mode was needed. The S_6 quadrature used a smallest polar angle of 22 degrees while the smallest S_{124} angle was 1.4 degrees.

*The quadrature order given here is that conventionally used and is not entirely consistent. The S_6 set contains 24 vectors distributed symmetrically and the S_{124} set contains 12 symmetrically distributed vectors directed downward and 94 vectors directed upward with many near the polar axis.

Figure 3* shows the dose rate in $\text{rad(c)}/\text{hr}$ from gamma radiation leaking from the top of the PVARA to a plane 37 meters above it. A void is assumed in the 37 meters to accentuate the differences between the results of the different methods. It is seen that the S_6 histogram method predicts values well below those of the S_6 smoothed and S_{124} , which agree very well for this case. The smallest S_6 angle intercepts this plane at about 1600 cm. from the axis. The histogram mode, then, includes the assumption that the particle current over the plotted range is the same as that expected at a much larger radius. The smallest S_{124} angle, on the other hand, intercepts this plane at about 90 cm. Since the source position has a range given by the 140 cm diameter of the reactor, any such underpredictions will be masked by compensating overpredictions. Since the S_6 smoothed results are produced by a curve fit which provides an extrapolation from the vector at 1600 cm, the excellent results are perhaps fortuitous. Poorer smoothed results would be expected when the angular flux values of the different S_N vectors varied more than in this case.

For a more difficult case, the radiation is considered which leaks from the side of the reactor and moves upward at a small angle with the side. The same three calculational modes were employed and transported through a void to a plane 3.4 meters above the reactor. This is approximately the location of the bottom of the propellant tank. These results are shown in Figure 4.

The detector plane in this calculation, at tank bottom, is close enough to the source locations to be intercepted by the vectors at the first two polar angles of the S_6 quadrature set. As a result, the oscillatory behavior of the histogram mode is exhibited and two peaks are seen which correspond to the two angles.

*While these data are obtained by collecting particles in radial interval bins, they are shown here by smooth curves in order to make comparisons easier.

GAMMA DOSE RATE FROM PVARA END AT PLANE
IN VOID 37 METERS ABOVE PVARA

Figure 3

Considering only those particles which can strike the bottom of the propellant tank, smoothing does not significantly improve the S_6 data. This is seen to be due to the difficulty of using data from larger angles to extrapolate to angles smaller than 22° from the side of the reactor. The side leakage at small angles can be considered further by extending the particles to the plane at 37 meters as was done for the top leakage. These results are shown in Figure 5.

As in the case shown in Figure 4, these results are for angles smaller than the S_6 vector nearest the polar axis and give an indication of the accuracy of the use of S_6 quadratures for a difficult application.

Coupling Internal to the S_N Problem

In considering the detail of small angle results from an S_{124} calculation, it appears that the intended detail of the problem may be extreme. Some scatter was observed in flux versus angle plots from the S_{124} calculation. With regard to the approximations inherent to an S_N calculation, such detail probably is not completely reliable. The loss of strict kinematic angle-energy relationship in using expansions in Legendre polynomials causes S_N calculations to predict some results in violation of energy-angle restrictions. As an example of this, the side leakage case was considered further in order to discover the origin of small angle radiation. The outer 2 centimeters of the PVARA is the aluminum pressure vessel wall. Because of the steep angle at which radiation from inside the wall must traverse the aluminum in order to be directed toward the plane at 37 meters, the low energy gammas are strongly attenuated.

GAMMA DOSE RATE FROM PVARA SIDE AT PLANE
IN VOID 3.4 METERS ABOVE PVARA

Figure 4

GAMMA DOSE RATE FROM PVARA SIDE AT PLANE
IN VOID 37 METERS ABOVE PVARA

Figure 5

To study the effect of the wall, S_N angular fluxes from the DOT code using an S_6 quadrature set were considered in the radial interval just inside the wall. The DASH code was then used to accomplish two calculations. First, DASH was used to sample particles in the direction of the 37 meter plane, attenuate them through the wall, and calculate their transport to the plane. This gives the dose rates at the plane from radiation which does not scatter in the wall. Second, DASH sampled particles in all outward directions into the wall and wrote these data on magnetic tape suitable for input to the COHORT Monte Carlo code. The wall was modeled in COHORT and the tape used as a source to calculate the transport of scattered gammas to the 37 meter plane. The results of these two calculations were summed* and compared with the S_6 smoothed and S_{124} calculations using angular fluxes at the outer surface of the wall. The energy spectra in a band at 400-500 cm on the plane are shown in Figure 6. The Monte Carlo result compares well with the S_{124} result over most of the energy range. Apparently the attenuation of the wall at very small angles cannot be properly accounted for in the S_6 calculation, resulting in a higher predicted dose rate. Probably the decoupling of angle-energy relationships in the S_N procedure hinders the assignment of scattered radiation to the lowest energy group, accounting for the steep drop in dose rate near zero energy. The peak at 6 to 7 Mev is due to γ sources in the beryllium reflector of the reactor.

In a similar application, an S_6 DOT calculation was used to produce angular flux information between the reactor core and reflector. The

*The effect of gamma sources in the wall was considered also, but did not contribute significantly to the total.

ENERGY DISTRIBUTION OF GAMMA RADIATION
 FROM PVARA SIDE IN 400-500 CM RADIAL BAND
 ON PLANE IN VOID 37 METERS ABOVE PVARA CENTER

Figure 6

particles simulated at this interface were traced through the reflector and wall regions by COHORT to a surface above the reactor, and a data tape of particle information produced. A pure Monte Carlo calculation of sources in the reflector and wall was also run using COHORT to produce a second data tape of particle information above the reactor. These data tapes were then used with a COHORT model of a propellant tank to calculate radiation levels at the top of the tank with different quantities of liquid hydrogen in the tank.

A similar set of calculations was performed using S_6 smoothed data at the outer surface of the reactor to produce a tape of particle information above the reactor. This tape was then used by COHORT to calculate radiation levels at the top of the tank with several different quantities of liquid hydrogen propellant in the tank. The results are compared for a particular hydrogen level in Figure 7. In this case, the tank has a capacity of about 180,000 lbs and is about 1/3 full. The top of the tank is about 30 meters from the top of the reactor. The results are divided into that radiation which does not scatter in the tank structure or contents (direct) and that which does scatter (scattered). These dose rates are consistent with earlier results in indicating the slight overprediction inherent in the S_6 data. Since leakage from the side of the reactor is the primary contributor to dose rate at the tank top, it is not surprising that the relationship between surface source and core-reflector interface source results should be similar to the relationship between the S_6 and S_{124} data seen earlier.

GAMMA DOSE RATE AT TANK TOP FROM PVARA SIDE
 SOURCES -- BASED ON S_6 DOT CALCULATION

Figure 7

Other Examples of the Method of Code Coupling

The use of the method is not limited, as we have seen, to using surface angular fluxes. Nor is it limited to tracing radiation through a void. Source data can be produced at any grid within the S_N problem, axially or radially. The data can be produced in the particle source format used by many Monte Carlo codes. (It has been used with FMC, COHORT and MORSE.) It can also produce tabular source data for FASTER or additional DOT problems.

Advantages of the Method of Code Coupling

The method allows considerable flexibility in choice of techniques to solve many complex radiation transport problems. It allows a user to take advantage of many of the special characteristics of S_N and Monte Carlo codes. Where the detail of Monte Carlo is needed, it can be employed. Where S_N is sufficient, it can be used with significant saving in computer time. Different degrees of detail are available in S_N by using tailored quadrature sets.

Any number of samples can be produced at a problem interface. As an example of the advantage of this, consider a problem of the type in which one determines the effect of scattering in the wall on the radiation level 37 meters away. A large number of particles scattering in the wall is necessary since few of the scattered particles reach detector regions offering small solid angles to the scattering region. If the particles must originate in a pure Monte Carlo sense, where the real particles originate, few ever arrive at the scattering region of interest. Thus a great many original particles would have to be produced in order to scatter a few in the wall.

But many scatters are necessary in the wall. Probably this problem would be prohibitively costly in computer time for all but the most liberally financed establishments. Using the S_N - Monte Carlo coupling technique, however,

the problem can be quite economical. A low quadrature S_N can be run on an IBM 360/65 in an hour or less for a 10-20 energy group, 50 x 30 spatial mesh problem. A high quadrature problem, such as an S_{124} , may take two to three times as long. The DASH problem to produce Monte Carlo data or calculate transport through a void or pure absorber takes five to 10 minutes. DASH can produce any required number of source particles. A Monte Carlo problem in the wall would take a few minutes longer. The whole process takes little more time than the original S_N . Furthermore, once the S_N problem has been run and the angular flux data saved on magnetic tape, it can be used any number of times. This allows additional analyses tailored to specific needs at any later time without repeating the bulk of the calculations. Later calculations can be performed in any degree of Monte Carlo employment, from pure S_N to pure Monte Carlo, with commensurate computer costs.

The coupling method is of general applicability and can be used to produce useful source data for any Monte Carlo analysis. It is most efficient for calculating radiation environment from shielded or distributed sources. Typical applications would be in calculating fluxes or dose rates in a void, air, or complicated three-dimensional structures from reactors or shielded isotopes.

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GLOSSARY

ADD	A code written at ANSC to add or modify Monte Carlo source data on magnetic tapes as used in coupling with DASH or for restarts of the Monte Carlo codes.
ANSC	Aerojet Nuclear Systems Company, Sacramento, California
COHORT	A system of Monte Carlo codes, S01, S02, H01, A01, A02, and A03 used extensively in NERVA radiation analyses.
COMMON	In a digital computer, that part of the active storage to which all subroutines of a computer code have access.
DASH	An original code written at ANSC in CY-1969 and extensively revised in CY-1970 to provide a wide range of code coupling and radiation transport capabilities.
DOT	A discrete ordinates transport code which uses the S_N method to calculate radiation transport in a two-dimensional array.
DOT-II	An updated version of the original DOT code. It has now largely replaced the original and is now normally referred to as DOT.
ENDF/B	A standard compilation of neutron cross-sections, the Evaluated Neutron Data File.
FASTER	A highly biased Monte Carlo code which has found limited application in NERVA radiation analyses. The code contains a convenient geometry description routine which has been incorporated into several other codes at ANSC.
FMC	A Monte Carlo code written in two versions: FMC-G for gamma ray transport and FMC-N for neutron transport. It was used at ANSC in early Monte Carlo calculations but has been replaced largely by the more flexible COHORT package.

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FMCPD	A code written at RRA to produce cumulative probability data from a magnetic tape of source data for the FMC Monte Carlo Code.
HIST1	The label on a data tape produced by the H01 code of the COHORT package. It contains source and collision data in the COHORT analysis.
IGLOO	A subroutine in the DASH code which describes the directions in which radiation transport is calculated by the DOT code.
MONDRIAN	A code written at ANSC to provide coupling data for DASH and DOT restart data within the boundaries of a DOT problem.
MORSE	A new multigroup Monte Carlo code which promises to be useful in a wide range of problems.
NERVA	The Nuclear Engine for Rocket Vehicle Application, a program administered by the Space Nuclear Systems Office, a joint office of the USAEC and NASA. Aerojet Nuclear Systems Company is prime contractor for the engine system and Westinghouse Electric Corporation is principal subcontractor responsible for the nuclear subsystem.
PARBIN	A code written at ANSC to provide distributed source information for DOT from COHORT histories which have reached thermal energies.
PVARA	Pressure vessel and reactor assembly of NERVA engine.
QAD	A point kernel code used at ANSC which uses the FASTER geometry description.
RRA	Radiation Research Associates, Fort Worth, Texas.
S_N	A calculational technique, as used in the DOT code, to calculate the distribution of radiation by the simultaneous solution of a set of equations.

SOTAG A code written at RRA to produce a magnetic tape of source data for the FMC Monte Carlo code from cumulative probability data.

Weight In Monte Carlo, that weighting factor applied to a single history or "particle". In pure Monte Carlo calculations it usually has a value between 0. and 1.0 and the total result is normalized by source strength and number of histories. In code coupling techniques, the weight has a value of a number of real particles per unit time and no source strength normalization is necessary. In discrete ordinates (S_N) the term is used to describe the solid angle associated with each quadrature angle.

APPENDIX

BIASING TECHNIQUES IN MONTE CARLO

By

J. H. Price and M. B. Wells

BIASING TECHNIQUES IN MONTE CARLO

In Monte Carlo calculations a large number of particle histories must be run in order that a sufficient number of particles will reach the region of interest to determine a statistical valid value of the average quantity of interest. As an example, consider a calculation to determine the energy, angle, and spatial distributions of the gamma flux penetrating the liquid hydrogen (LH_2) contained in a typical NERVA configuration.¹ In calculations of this type, much of the computer run time can be spent in tracing the particle history in the LH_2 region near the origin of the radiation source. Here the probability of the particle eventually reaching the region of interest is very low. Thus, to obtain an acceptable average particle behavior within a reasonable computer run time it is necessary to use biasing or importance sampling to increase the probability of the particles reaching the region of interest.

It should be noted that the efficiency of a Monte Carlo calculation is related to the biasing technique selected for use in a particular problem and the amount of effort required to determine the optimum values of the biasing parameters. In most applications this selection is usually based on past experience only. If no other basis for selection is available, this method should be used. In general, if biasing is necessary, the efficiency of the calculations is greatly increased regardless of the value of parameters used. If the radiation analysis problem involves an extraordinary amount of attenuation, then an initial investigation is desirable to determine the optimum biasing techniques and biasing parameters to obtain maximum efficiency.

As a result of the potential savings in computer time and the possible increased accuracy of the results that could be obtained when using importance sampling techniques, work has been carried out in two related areas over the past year. The two areas of work include:

- 1) An investigation of the application of the biasing techniques presently existing in FMC and COHORT and the development of a method of computing the biasing parameters associated with use of the exponential transformation so as to produce optimum biasing for NERVA type applications.

- 2) The development of a useful method of using the adjoint function to define biasing information in a Monte Carlo procedure with emphasis on the implementation of the method in the COHORT procedure.

These areas of work are discussed below.

3.1 Existing Biasing Techniques in FMC and COHORT

The FMC⁴ and COHORT³ Monte Carlo procedures have several different biasing techniques available. The usefulness or importance of each of these techniques is dependent on the geometry and radiation source being employed in the Monte Carlo calculations. Also, to use the technique properly, it is necessary to have some knowledge of the biasing parameters that should be used with each technique. A typical NERVA configuration¹ was used in a number of different calculations to determine the effectiveness of each biasing technique and to obtain some knowledge of the proper biasing parameters to be used.

The calculations employed the PDL source and the problem geometry contained the PVARA and the LH₂ tank of a typical NERVA configuration. The objective of the investigation was to determine the optimal biasing parameters and the usefulness of the techniques to increase the number of particles per unit run time being transported through the liquid hydrogen and the LH₂ tank. These calculations are similar to those made in a previous study¹¹ to determine the energy, angle, and spatial distributions of the gamma flux at a plane positioned above the LH₂ in the tank.

Biasing techniques in FMC include 1) acceleration factors, 2) splitting and Russian Roulette, and 3) exponential transformation. Acceleration factors or energy group constants may be used to obtain favorable sampling from the source spectrum. Particle splitting (i.e., an increase or decrease in the number of particles in a cluster) may be used at region boundary crossings, or change in energy, and on change in location, direction and energy at collision points. The exponential transformation may be used to adjust the mean-free-path length (i.e., increase or decrease)

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in any of six directions for a given region. The extent of the adjustment and the direction may be different for each region. The particle weights are adjusted for each of the techniques to account for the bias introduced. The exponential transformation is the only optional variance reduction technique provided in COHORT.

The initial calculations were made using exponential transformation in the regions of the defined geometry that contained LH_2 . The calculations were made for biasing parameters such that a LH_2 level of 38,800 lbs. represented an equivalent thickness of approximately 3 mean-free paths (MFP) along the tank centerline for a 1.0 Mev gamma. The LH_2 region without biasing had an approximate thickness of 7 MFP. A calculation was also made in which no exponential transformation was used. These results were used as a basis of comparison. The results from these calculations showed that the use of the exponential transformation gave an increase of a factor of 5 in the number of particles per unit time that reached the plane of interest above the LH_2 . Thus, the use of the exponential transformation proved to be very beneficial in calculations of this nature.

Two different splitting techniques were tried in similar calculations. The region importance technique is a means of particle splitting on location at region boundary crossings. This is accomplished by means of region importances that are specified in the program input. For the calculations, a region importance of three was assigned to the LH_2 regions with all other regions having an importance of one. This technique showed no increase per unit run time in the number of transmitted particles.

The second technique called fine splitting, evolved splitting on change in location, direction, and energy at collision points. The degree of splitting is designated by input quantities that must be specified for each region and energy group. The direction of interest is also specified in the input. All computer runs employing fine splitting were terminated due to a computer time limit and no results were obtained. In an attempt to determine a reason for the long run times, an inspection of the fine splitting routines in FMC indicated that errors exist which would require additional checkout and modifications beyond the scope of this investigation.

Appendix

The biasing technique using acceleration factors consist only of a simple means of altering the input source spectrum within the program. No calculations were made assuming an altered source spectrum.

From the results of these calculations, it was concluded that of the biasing techniques available, only the exponential transformation should be used in NERVA analysis where the number of particles that penetrate such components as the LH₂ tank or an engine disk shield is important. The exponential transformation option is available in both FMC and COHORT. The values of the optimum biasing parameters to be used in the exponential transformation are highly dependent on the problem geometry and the radiation source. It is not feasible, therefore, to calculate in advance the optimum biasing parameters for all future NERVA applications. Thus, a computer code designated BIPAR was written to calculate optimum values of the exponential transformation parameters once the problem geometry and radiation source have been defined.

The exponential transform is a form of importance sampling employing an altered transport kernel that is specified by an importance function. It has been shown^{12, 13, 14}, that the importance function can very readily be represented by the adjoint solution. The BIPAR code was written to calculate from the adjoint solution the necessary parameters in the proper format for input in the FMC and COHORT Monte Carlo codes. These parameters are used by the Monte Carlo codes to defined the altered transport kernel.

In COHORT the exponential transformation biasing parameter $B(R')$, which is region dependent only, is used to define the pseudo total cross section

$$\bar{\Sigma}_T(E, R') = \Sigma_T(E, R') (1 - B \cdot D) \quad (3.1)$$

where $\bar{\Sigma}_T(E, R')$ is the total macroscopic cross section as a function of energy for region R and D is the direction cosine for the direction in which biasing is to be applied. When $\cos^{-1}D$ is greater than 90° , COHORT sets $\bar{\Sigma}_T(E, R') = \Sigma_T(E, R')$. B is a biasing parameter which can take on values between 0 and 1.

Appendix

In FMC a pseudo mean-free-path distance λ^r is input which is region dependent but not energy dependent. It is used to determine a pseudo total macroscopic cross section, $\bar{\Sigma}_T(E, R')$ with which distances between collisions are determined. In FMC, $\bar{\Sigma}_T(E, R')$ is defined in terms of λ^r by the equation

$$\bar{\Sigma}_T(E, R') = \frac{D}{\lambda^r} + (1-D)\Sigma_T(E, R') \quad (3.2)$$

The BIPAR code was written for the purpose of obtaining optimum values of the parameter B and λ^r from a knowledge of the adjoint flux. It assumes that the adjoint flux has previously been calculated with use of the ANISN code¹⁵, which is a one dimensional transport procedure. Therefore, it is assumed that a one-dimensional importance function can be used to represent a three-dimensional problem.

The use of the one-dimensional adjoint flux limits the geometrical configurations that are meaningful. In BIPAR, all configurations are assumed to have azimuthal symmetry about the Z axis and to consist of layers or slabs bounded by surfaces of revolution such as a cylinder, cone, or hemisphere. The calculation of $B(R')$ for each region is made with respect to a representative point located on the Z axis at the center of each layer or region. The direction of motion is given by the direction cosine measured with respect to the Z axis.

The importance function for the exponential transformation is assumed to vary exponentially in the direction of importance. This importance function is to be specified by the adjoint flux. Thus the assumption is made that the adjoint flux along the particle track may be represented by an exponential of the form

$$V(R, E, D) = \text{EXP}[S(R, E, D)|\vec{r}' - \vec{r}|] \quad (3.3)$$

where $S(R, E, D)$ is the slope of the function specifying the adjoint flux with energy E and direction D in region R' and $|\vec{r}' - \vec{r}|$ is the distance along the particles path from the previous collision point in the direction of motion. The region R is defined as the region containing the position $\vec{r}$.

The slopes $S(R', E, D)$ for discrete intervals in E and D are calculated from the adjoint flux by the use of the method of least squares. The exponential transformation parameter $B(R', E, D)$ is then computed from the equation

$$B(R', E, D) = \frac{[S(R', E, D)]}{[D\Sigma_T(R', E)]} \quad (3.4)$$

If the particle track passes through only one region, then the importance function is assumed to be undefined for that region, i.e., $B(R', E, D) = 0$ for that region.

Since the exponential transformation parameter used for input to COHORT is a function of region only, it is necessary that an average value of $B(R')$ be computed for each region. This is accomplished by first computing $B(R', D)$ with the equation

$$B(R', D) = \frac{\int B(R', E, D) V(R', E, D) dE}{\int V(R', E, D) dE} \quad (3.5)$$

and then $B(R')$ with the equation

$$B(R') = \text{EXP} \left[\frac{\sum_{D=D_1}^{D_N} B(R', D) - S_B \sum_{D=D_1}^{D_N} (1-D)}{N} \right] \quad (3.6)$$

where S_B is the slope of $B(R', D)$, D_i is the direction cosine of the i th direction of motion, and N is the number of different directions at which $B(R', D)$ was calculated. If $B(R', D)$ was calculated for only one direction D_j at which $B(R', D) \neq 0.0$, then $B(R')$ is set equal to $B(R', D_j)$. If the calculations for region R' were such that $B(R', D) = 0.0$ for all directions of motion, the $B(R')$ is set equal to zero.

In problems where deep penetration is necessary, it is often advantageous for the particle path lengths to be selected such that the particles do not penetrate beyond the limits of the slab. These limits are defined by a certain $Z_{\max}$ (i.e., a maximum Z coordinate). This means that if the exponential transformation is used to enhance penetration, it should be used to a lesser degree as the particles collision point approach $Z_{\max}$. In the COHORT and FMC codes there are no options to allow such conditions to be applied directly. Thus, it is necessary to adjust the exponential transformation parameters that are input into the codes.

Appendix

If a linear variation of $B(R')$ is assumed across the slab, then the normalized function $B_N(R')$ is given by the equation

$$B_N(R') = B(R') \left[\frac{Z_{\max} - Z(R')}{THKS} \right] \quad (3.7)$$

where $Z(R')$ is the coordinate of the point in region R' for which $B(R')$ was determined, THKS is the total thickness of the layers or slab (i.e., $Z_{\max} - Z_{\min}$) and $Z_{\max}$ is the maximum Z coordinate of the slab.

The parameter λ^r as used in FMC is computed by use of the equation

$$\lambda^r(R') = \frac{1}{\Sigma_T'(R') (1 - R')} , \quad (3.8)$$

where $\Sigma_T'(R')$ is computed from the equation

$$\Sigma_T'(R') = \frac{\int \Sigma_T(R', E) V(R', E, A) dE}{\int V(R', E, A) dE} . \quad (3.9)$$

The parameter A is the direction cosine of the direction nearest the direction of interest at which the adjoint flux is known.

A normalized value of $\lambda_N^r(R')$ can also be obtained from the equation

$$\lambda_N^r(R') = \frac{1}{\Sigma_T'(R') (1 - B_N(R'))} \quad (3.10)$$

The printout obtained from the BIPAR code gives a listing of the parameters $B(R')$, $B_N(R')$, $\lambda^r(R')$ and $\lambda_N^r(R')$ as a function of the region number R' .

3.2 Importance Sampling Using the Adjoint Flux

The work described in this section is a continuation of the studies performed for ANSC under Task III of Purchase Order NP-000179. In the previous study it was shown that through the use of importance sampling based on the adjoint function it is possible to obtain significant gains in the efficiency of a Monte Carlo calculation. It was also noted that implementation of this form of importance sampling would be easier to accomplish in COHORT than in the other Monte Carlo procedures used at ANSC. It was recommended that COHORT

be modified to include a systematic application of the adjoint flux in selecting collision sites, energies, and directions from the transport and scattering kernels of the integral transport equation. The present work describes the development of a method of selecting the necessary parameters from an altered kernel specified by the adjoint function. This includes the development of a method for determining the necessary information in the proper format to specify the altered kernels. The object of this work is to be able to incorporate into the transport and collision kernels as much of the adjoint function as possible, without significantly increasing the computer time necessary to sample from the altered kernels.

It should also be noted that much of the theory described below is similar to that developed by Burgart¹⁶ for neutron transport in the 05R code. The following theory is limited to gamma-ray transport within the COHORT procedure. It was noted by Burgart that most of his investigation is applicable to gamma-ray transport.

3.2.1 The Transport Equation

The conservation equation for particle transport is given by the expression

$$X(P)dP = S(P)dP + \int dP' X(P') K(P' \rightarrow P) dP \quad (3.11)$$

where dP is an incremental volume in phase space about the point P and

- $X(P)dP$ = the expected number of particles from collisions or sources, which are leaving the volume element dP ,
- $S(P)dP$ = the expected number of particles which are created within the volume dP by extraneous sources,
- $K(P' \rightarrow P)dP$ = the expected number of particles which have collisions in dP and come from collisions which occurred at phase space position P' .

Particles which leave sources at positions P' are included in the $K(P' \rightarrow P)dP$ term and may be thought of as zeroth order collisions.

Usually the term $K(P' \rightarrow P)$ is split into two multiplicative factors as follows:

$$\begin{aligned} K(P' \rightarrow P) dP &= K(E' \rightarrow E, \vec{r}' \rightarrow \vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) dE d\vec{r} d\vec{\Omega} \\ &= T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) dE d\vec{r} d\vec{\Omega}. \end{aligned} \quad (3.12)$$

The term $T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r})$ is the usual transport kernel and $C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$ is the corresponding collision kernel. C may or may not be a function of the position vector $\vec{r}$ depending upon the variation of material or cross sections with respect to position. If cross sections are constant for all $\vec{r}$, then the $\vec{r}$ dependence of C is removed. Using T and C the transport equation may be rewritten as follows

$$\begin{aligned} X(\vec{r}, E, \vec{\Omega}) d\vec{r} dE d\vec{\Omega} &= S(\vec{r}, E, \vec{\Omega}) d\vec{r} dE d\vec{\Omega} + \\ &\int \int \int d\vec{r}' dE' d\vec{\Omega}' X(\vec{r}', E', \vec{\Omega}') T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) d\vec{r}' dE' d\vec{\Omega}'. \end{aligned} \quad (3.13)$$

If one wishes to obtain the quantity λ , then

$$\lambda = \int \int \int F(\vec{r}, E, \vec{\Omega}) X(\vec{r}, E, \vec{\Omega}) d\vec{r} dE d\vec{\Omega} \quad (3.14)$$

where λ may be referred to as an eigenvalue and $F(\vec{r}, E, \vec{\Omega})$ is the response function for λ . Depending on the form of $F(\vec{r}, E, \vec{\Omega})$, λ may be fluence, current, dose, energy fluence, or energy current. The integral for λ is usually obtained by the use of statistical estimation as part of the Monte Carlo calculation.

3.2.2 Importance Sampling and Adjoint Formulation

If randomly chosen variables are selected using probability density functions other than those defined by K , then the selections are said to be biased. Equation (3.11) can be written

$$X(P) = S(P) + \int X(P') K^*(P' \rightarrow P) \frac{K(P' \rightarrow P)}{K^*(P' \rightarrow P)} dP' \quad (3.15)$$

$$= S(P) + \int X(P') K^*(P' \rightarrow P) W(P' \rightarrow P) dP' \quad (3.16)$$

where $W(P' \rightarrow P)$ is a weighting factor that must be applied to account for the use of K^* instead of K .

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Note that the object of importance sampling is to choose K^* such that the energy, direction, and spatial position are selected to insure an increased probability of the particle making a contribution to the answer of interest. Thus, an appropriate expression for K^* can be written

$$K^*(P' \rightarrow P) = K(P' \rightarrow P) \frac{I_K(P)}{I_K(P')} \quad (3.17)$$

where $I_K(P)$ is the importance function.

The application of K^* will be no better than use of the original equations unless the arbitrary function $I_K(P)$ is chosen such that it reduces the variance of λ (Eq. 3.14) is for a given sample size. If a judicious choice of $I_K(P)$ is made such that particles will be transported to regions near points of interest, then the desired results will occur. The selection of parameters according to their importance in contributing to the desired answer, lends the name of "importance function" to $I_K(P)$.

One method of obtaining a function which is a reasonable choice for $I_K(P)$ is through the use of the adjoint formulation of the original problem. The adjoint formulation may be written as follows:

$$V(P)dP = F(P)dP + \int dP' K(P \rightarrow P') V(P')dP \quad (3.18)$$

and

$$\lambda = \int S(P)V(P)dP \quad (3.19)$$

where λ is the same eigenvalue as obtained from Equation (3.14).

$V(P)dP$ may be interpreted as the expected contribution to λ of particles emerging from collisions in dP about P . Hence, $V(P)$ should always be a reasonable choice of $I_K(P)$.

If Equations (3.18) and (3.19) could be solved exactly, then there would be no need to pursue the problem further since the eigenvalue λ would be known. Since the same geometrical conditions exist for the application of these equations as exist for the application of Equations (3.13) and (3.14), Equations (3.18) and (3.19) cannot in general be applied to problems which contain complicated geometrical constraints. However, the adjoint equations could be applied to a simplified problem whose geometrical configuration has the same characteristics as that of a more complicated problem.

Then the solution of the adjoint equation for the simplified geometry should yield a function which would be a good choice for the importance function to be used in the Monte Carlo calculation for the more complicated geometry.

It must be noted that the importance function $I(E, \vec{r}, \vec{\Omega})$ is defined for a given value of the response function, which, in turn, fixes the spatial location for which λ is to be evaluated. If λ is to be evaluated at more than one spatial position, then it is highly unlikely that acceptable results would be obtained for those receiver positions for which the optimum importance function differed significantly from the importance function used in the Monte Carlo calculation.

To make use of the full adjoint it would be highly desirable to have a means of selecting collision sites and energies and directions of motion after collision. To do so means that one make use of the spatial, energy, and direction parameters defined by the adjoint $V(\vec{r}, E, \vec{\Omega})$.

Let us examine the function $K^*(P' \rightarrow P)$ for the case of a three-dimensional geometry. Define the following

$$T^*(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) = \frac{T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) \left[\frac{I(E', \vec{r}, \vec{\Omega}')}{I(E', \vec{r}', \vec{\Omega}')} \right]}{\int T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) \left[\frac{I(E', \vec{r}, \vec{\Omega}')}{I(E', \vec{r}', \vec{\Omega}')} \right] d\vec{r}} \quad (3.20)$$

and

$$C^*(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) = \frac{C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \left[\frac{I(E, \vec{r}, \vec{\Omega})}{I(E', \vec{r}, \vec{\Omega}')} \right]}{\iint C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \left[\frac{I(E, \vec{r}, \vec{\Omega})}{I(E', \vec{r}, \vec{\Omega}')} \right] dE d\vec{\Omega}} \quad (3.21)$$

From Equation (3.12) it follows that $K^*(P' \rightarrow P)$ is given by the equation

$$K^*(E' \rightarrow E, \vec{r}' \rightarrow \vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) = T^*(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) C^*(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}). \quad (3.22)$$

Note that T^* and C^* are properly normalized probability density functions such that

$$\iiint K^*(E' \rightarrow E, \vec{r}' \rightarrow \vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}) dE d\vec{r} d\vec{\Omega} = 1. \quad (3.23)$$

Equations (3.20) and (3.21) may also be written as

$$T^*(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) = \frac{T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) I(E', \vec{r}, \vec{\Omega}')}{\int T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) I(E', \vec{r}, \vec{\Omega}') d\vec{r}}, \quad (3.24)$$

and

$$C^*(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) = \frac{C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) I(E, \vec{r}, \vec{\Omega})}{\int \int C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) I(E, \vec{r}, \vec{\Omega}) dE d\vec{\Omega}}. \quad (3.25)$$

Thus, the collision site $\vec{r}$ can be selected from the altered transport kernel specified by the importance function $I(E', \vec{r}, \vec{\Omega}')$ which is dependent on the energy and direction after the previous collision. Also, the energy E , and direction after collision, $\vec{\Omega}$, may be selected from the altered collision kernel specified by the importance function $I(E, \vec{r}, \vec{\Omega})$ which is dependent only on the collision position, $\vec{r}$.

Equation (3.25) shows that the altered kernel is the product of the true scattering distribution and the importance function. The scattering distributions for gamma rays are expressed in terms of the particle direction before collision. The importance function is most often expressed in terms of a fixed coordinate system such as that used in the COHORT procedure. The importance function and the scattering distribution must be expressed in the same coordinate system. This may be done using the spherical triangle formula. However, this change of coordinate system leads to very complicated expressions for the altered kernel, and the selection of the scattering angle cannot be performed efficiently using standard methods.^{17,18,19} Burgart¹⁶ defines a method of incorporating angular biasing (i.e., selecting the scattering angles from an altered kernel specified by an importance function) in three-dimensional Monte Carlo calculations. The method involves the introduction of an angular grid with discrete directions fixed in the laboratory coordinate system along which the particles are required to travel. Once the appropriate scattering probabilities and values of the importance function have been determined for each discrete direction, a discrete scattering distribution may easily be determined. The scattering angle may then be selected from the resulting biased distribution using standard techniques. The use of the discrete angular grid in the selection of particle track lengths from Equation (3.24) is also very

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useful. The track lengths may be biased independently for each discrete direction. In most earlier methods the importance functions applied only in a single direction and the resulting track lengths were adjusted to account for variations in the particles direction from the fixed direction. The altered kernels are described below with respect to the actual calculations necessary to determine the proper probability distributions and the application of each in the COHORT procedure.

3.2.3 The Altered Transport Kernel

The exponential transformation is an importance sampling scheme in which the importance function is represented by an exponential. The importance function is used to alter the transport kernel resulting in an expression similar to Equation (3.24). A simple form of the importance function and one that is similar to that presently employed in COHORT is given by the equation

$$I(E', \vec{r}, \vec{\Omega}') = e^{B(E', \vec{r}', \vec{\Omega}') - \Sigma_t(E', \vec{r}') |\vec{r}' - \vec{r}|} \quad (3.26)$$

where $B(E', \vec{r}', \vec{\Omega}')$ is the parameter used to define the importance function, $\Sigma_t(E', \vec{r}')$ is the total cross section at the energy E' and, $\vec{r}'$ and $\vec{r}$ are the position vectors of the previous interaction and the particle, respectively.

Note that in COHORT the parameter to define the importance function is not dependent on energy or direction as is $B(E', \vec{r}', \vec{\Omega}')$. The transport kernel $T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r})$ is given by the equation

$$T(E', \vec{\Omega}', \vec{r}' \rightarrow \vec{r}) = \Sigma_t(E', \vec{r}') e^{-\Sigma_t(E', \vec{r}') |\vec{r}' - \vec{r}|} \quad (3.27)$$

which is the same kernel as presently used in COHORT. Thus, in using the transport equation and importance function given in Equations (3.27) and (3.26), respectively, the biased gamma track lengths, $\ell = |\vec{r}' - \vec{r}|$, may be selected in the same manner as previously employed in COHORT. In the notation used in COHORT, this would be the selection of ℓ from the product of the two exponentials which results in the equation

$$\ell = \frac{-\ln RN}{\Sigma_t(L', R') [1 - B(E', R', N)]} \quad (3.38)$$

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where N denotes the direction of the gamma, $\vec{\Omega}'_N$, in material region R' , and RN is a random number between zero and one.

The unit vector, $\vec{\Omega}'_N$, is along one of the fixed discrete directions in which gammas are allowed to scatter. The region R' is a discrete mathematical region defined in the COHORT input. This form of the exponential transform not only makes it easy to select from the altered transport kernel but also requires only one parameter $B(E', R', N)$ for a given energy, direction, and region.

As noted above, to obtain an optimum importance function the necessary parameters should be specified by the adjoint function. A method for calculating the $B(E', R', N)$ parameters from the numerical adjoint is described below. The listing of subroutine source decks that may be incorporated into the H01 routine of COHORT to calculate the necessary parameters is given in Appendix A. These routines will not stand alone as they use some of the subroutines presently employed in the COHORT routines.

The importance function for the exponential transformation as defined by Equation (3.26) is assumed to vary exponentially in the direction $\vec{\Omega}'$. This importance function is to be specified by the adjoint flux defined in some previous calculations. The assumption is made that the adjoint flux along the direction $\vec{\Omega}'$ may be represented by an exponential of the form

$$V(E', \vec{r}, \vec{\Omega}') = e^{S(E', \vec{r}, \vec{\Omega}') \ell} \quad (3.29)$$

where $S(E', \vec{r}, \vec{\Omega}')$ is the slope of the function defining the adjoint flux associated with a particle that has undergone a collision at $\vec{r}'$ and,

ℓ is the particle track length or distance measured along $\vec{\Omega}'$ between $\vec{r}$ and $\vec{r}'$.

By determining $S(E', \vec{r}, \vec{\Omega}')$ for each energy E' and spatial position $\vec{r}'$, it is possible to determine the function for the adjoint flux along each of the fixed directions the particles are allowed to travel. This function is then used to determine the importance function in the exponential

transformation according to the equation:

$$B(\vec{E}', \vec{r}', \vec{\Omega}') = \frac{S(E', \vec{r}', \vec{\Omega}')}{\Sigma_t(E', \vec{r}')} \quad (3.30)$$

In Equations (3.29) and (3.30), the energy E' is most often the mid-point of an energy group which is part of a multigroup structure. Also, in terms of the discrete mathematical regions used within a Monte Carlo code, the spatial position of a interaction will be specified by an R' instead of $\vec{r}'$. Each region R' is defined by mathematical boundaries. These regions are combined to make a mathematical model.

If the numerical adjoint flux is known for a group of regions, the slope of the adjoint flux $S(E', R', \vec{\Omega}')$ along each direction may be calculated for each direction by the method of least squares from the equation

$$S(E', R', \vec{\Omega}') = \frac{\sum_{I=R'}^R L(I) V(E', I, \vec{\Omega}') - \sum_{I=R'}^R L(I) \sum_{I=R'}^R V(E', I, \vec{\Omega}')}{\sum_{I=R'}^R [L(I)]^2 - \left[\sum_{I=R'}^R L(I) \right]^2} \quad (3.31)$$

where N is the number of mathematical regions through which the vector $\vec{\Omega}'$ would pass before entering a region for which V was not defined, and

$L(I)$ is the distance along $\vec{\Omega}'$ through region I .

The other terms are as defined above. In Equation (3.31) if $N < 2$ the expression should be set to zero for that region, energy and direction. The use of Equations (3.30) and (3.31) in the Monte Carlo codes is given in Subsection 3.2.7.

3.2.4 The Altered Collision Kernel

The altered collision kernel is given by Equation (3.25). As noted earlier, direct selection of the scattering angle and energy from this kernel is very difficult to accomplish. The difficulty arises from the fact that the importance function and the scattering distribution are specified relative to two different coordinate systems. To overcome these

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difficulties and to introduce a more general method of incorporating angular biasing, a discrete angular grid, fixed in the laboratory coordinate system is introduced. In this method, the particle is required to travel in one of the specified directions. A set of thirty directions were obtained by connecting the center of an icosahedron with the midpoints of the edges. This set of directions has the useful property that only nine different scattering angles exist; that is, for any of the thirty incoming directions only nine different polar angles are necessary to describe scattering to any of the thirty possible outgoing directions. Once the nine scattering probabilities are determined and the direction of the incoming particle is given, the probability of scatter to each of the thirty directions may easily be obtained. Furthermore, if the problem has azimuthal symmetry, only nine values of the importance function may be necessary to determine the values for all thirty directions. It should also be noted that equal solid-angle increments are associated with each of the thirty directions.

For gamma ray transport in COHORT, the interactions considered include pair production, photoelectric and Compton scattering. Photoelectric events are not permitted and the weight of the particles are adjusted to account for the exclusion of this absorption process. Pair production events are assumed to result in two 0.51 MEV gammas with an isotropic distribution. For the Compton scattering events, a unique relationship between the incoming energy, the scattering angle, and the outgoing energy is given by the equation

$$E = \frac{E'}{1 + \frac{E'}{0.511} (1 - \cos \psi)} \quad (3.32)$$

where $\cos \psi$ is equal to the cosine of the angle between $\vec{\Omega}'$ and $\vec{\Omega}$.

If we let each of the discrete directions be specified by an index j , the selection of an outgoing direction and energy becomes a selection of j and E given j' and E' . Equation (3.25) may be rewritten

$$C^*(\vec{r}, E, j \rightarrow j) = \frac{C(\vec{r}', E', j' \rightarrow j) \int (E, \vec{r}, j) \Delta\bar{\Omega}_j}{\sum_{j=1}^{30} C(\vec{r}', E', j' \rightarrow j) \int (E, \vec{r}, j) \Delta\bar{\Omega}_j} \quad (3.33)$$

where $\Delta\bar{\Omega}_j$ is the solid angle associated with the j^{th} direction. The

distribution given by Equation (3.33) may now be selected from directly using the following procedure. First, the energies associated with each outgoing direction are determined from Equation (3.32). The importance function is then evaluated for each outgoing direction and appropriate energy, and the altered collision kernel given by Equation (3.33) normalized. Using techniques presently employed in COHORT the outgoing direction is then selected from the discrete probability density function given by Equation (3.33) and the outgoing energy is determined from Equation (3.32). This procedure for selecting outgoing directions and subsequently outgoing energies allows the importance function for each outgoing direction to be evaluated at the appropriate outgoing energy, rather than at the incoming energy.

The gamma ray scattering distribution for a Compton event may be obtained from the Klein-Nishina formula by use of the equation

$$P(E', \psi) = \frac{\frac{d\sigma}{d\Omega}(E', \psi)}{\sigma_c(E')} = \frac{r_o^2}{2} \left[\frac{(E/E') + (E/E')^3 - (E/E')^2 \sin^2 \psi}{\sigma_c(E')} \right] \quad (3.34)$$

where r_o is the classical electron radius, and

$\sigma_c(E')$ is the gamma scattering cross section per electron at energy E' .

The cross section $\sigma_c(E')$ is given by the equation

$$\sigma_c(E') = 2\pi r_o^2 \left\{ \frac{1+Q}{Q^3} \left[\frac{2Q(1+Q)}{1+2Q} - \ln(1+2Q) \right] + \frac{1}{2Q} \ln(1+2Q) - \frac{1+3Q}{(1+2Q)^2} \right\}$$

Where $Q = E'/0.511$ for gamma energy in units of MEV.

For the distribution given in Equation (3.34) it is necessary to determine the scattering probabilities for the nine scattering angles of the discrete angular grid. In terms of the Monte Carlo code, the probabilities must be representative of the solid angle $\Delta\vec{\Omega}_j$ which is defined by $\cos \psi_j$ and $\cos \psi_{j+1}$ and the direction specified by j . The angle ψ_{j+1} is

$$\psi_{j+1} = \cos^{-1} \left[\frac{\cos \phi_j + \cos \phi_{j+1}}{2} \right] \quad (3.36)$$

where ϕ_j is the j^{th} scattering angle defined by the discrete grid. Also, the probabilities must represent some energy group structure, usually

multigroup, whose limits are designated by $\bar{E}_n$. The discrete probability distribution for each energy and angle group which are specified by n and j , respectively, may be calculated from the equation

$$P(n, j) = \frac{\int_{\cos\psi_j}^{\cos\psi_{j+1}} \frac{d\sigma}{d\Omega}(n, \psi_j) \sin\psi d\psi}{\int_{-1}^{+1} \frac{d\sigma}{d\Omega}(n, \psi_j) \sin\psi d\psi} \quad (3.37)$$

where

$$\frac{d\sigma}{d\Omega}(n, \psi_j) = \frac{\int_{E_n}^{E_{n+1}} \frac{d\sigma}{d\Omega}(E', \psi_j) \sigma_c(E') dE'}{\int_{E_n}^{E_{n+1}} \sigma_c(E') dE'} \quad (3.38)$$

If the interaction is a pair production event, the distribution which is independent of energy E_n is given by the equation:

$$P(j) = \frac{\Delta\Omega_j}{4\pi} \quad (3.39)$$

Once the necessary scattering distributions (i.e., $C(\vec{r}, \bar{E}', \psi_j)$) have been determined from Equations (3.37) and (3.39) and the importance function $I(\bar{E}, \vec{r}, j)$ is represented by the adjoint flux $V(\bar{E}, \vec{r}, j)$, it is a simple calculation to determine the altered scattering distributions from the altered kernel given by Equation (3.33). A listing of the subroutine source deck necessary to determine the scattering distribution from Equation (3.33) is given in Appendix B. The distributions are determined for discrete mathematical regions for which the adjoint flux is known.

3.2.5 The Discrete Angular Grid

The thirty discrete directions of the angular grid were obtained by connecting the center of an icosahedron with the midpoint of the edges. Each of the directions are described in detail in Table 1. Shown are the polar or scattering angle and the azimuthal angles which are measured with respect to the + Z- and + Y-axes, respectively. Also shown are the direction cosine of each angle. The direction cosines α , β , and γ are measured with respect to the X, Y, and Z axes, respectively.

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Table 1. The Discrete Angular Grid

Scattering Angle Number	Polar Angle (deg)	Azimuthal Angle (deg)	Alpha	Beta	Gamma
1	0	0	0.000	0.000	1.000
2	36	60	0.294	0.500	0.809
		120	-0.294	0.500	0.809
		240	-0.294	-0.500	0.809
		300	0.294	-0.500	0.809
3	60	30	0.750	0.433	0.500
		150	-0.750	0.433	0.500
		210	-0.750	-0.433	0.500
		330	0.750	-0.433	0.500
4	72	60	0.475	0.823	0.309
		120	-0.475	0.823	0.309
		240	-0.475	-0.823	0.309
		300	0.475	-0.823	0.309
5	90	0	1.000	0.000	0.000
		90	0.000	1.000	0.000
		180	-1.000	0.000	0.000
		270	0.000	-1.000	0.000
6	108	60	0.475	0.823	-0.309
		120	-0.475	0.823	-0.309
		240	-0.475	-0.823	-0.309
		300	0.475	-0.823	-0.309
7	120	30	0.750	0.433	-0.500
		150	-0.750	0.433	-0.500
		210	-0.750	-0.433	-0.500
		330	0.750	-0.433	-0.500
8	144	60	0.294	0.500	-0.809
		120	-0.294	0.500	-0.809
		240	-0.294	-0.500	-0.809
		300	0.294	-0.500	-0.809
9	180	0	0.000	0.000	-1.000

3.2.6 The Adjoint Flux Calculation

The numerical adjoint flux required in Equations (3.31) and (3.33) may be determined by several methods. One method often used^{16,20} is the one-dimensional discrete ordinates code ANISN.¹⁵ The ANISN calculations should be made with the Monte Carlo estimator of the answer of interest as the source term. The source should be located at a similar position to that of the point of interest in the Monte Carlo calculation. Because the results are for a one-dimensional calculation, they must be extended to three-dimensions for use in the Monte Carlo calculations. This may be done using methods similar to those employed in the DASH procedure.⁶ This is the one area in which further work is needed. Additional work should be done in this area to develop a routine or subroutine to take the one-dimensional adjoint and extend it to a representative three-dimensional adjoint in the proper energy and angle groups.

3.2.7 Implementation of Adjoint Biasing in COHORT

The subroutines listed in Appendices A and B were written to be incorporated into the COHORT procedure as described in Reference 3. Described below to aid in the implementation of the subroutines in H01 of the COHORT procedure are 1) the information that must be transferred into each subroutine from the H01 subroutines, 2) the CALL statement required in H01 for each subroutine, 3) when and where each subroutine should be called and 4) the output of each subroutine.

First consider the subroutine given in Appendix A that was written to calculate the necessary exponential transformation parameters. The subroutine BIPAR should be called only one time. It should be called at the start of subroutine HIGENE after all input data have been read. The CALL statement should have the format:

```
CALL BIPAR (NRGWB, NREG, NMGEG, MBD, S(LV),S(LY), S(LZ), S(MA), S(MC), S(ME),
           S(MF), S(MR), S(MS), S(MT), S(MU), S(MV), S(MW), S(MX), S(MY), S(1),
           S(2), S(LA), S(LW), MS).
```

The S(XX) terms in the above statement are the storage address in the S-array or the dimensioned variables used in subroutine BIPAR. The storage locations not previously defined in COHORT are defined as follows:

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```

MR = MQ + NELG
MS = MR + 30*NMGEG*NRGWB
MT = MS + NREG
MU = MT + 30*NMGEG*NRGWB
MV = MU + NREG
MW = MV + NREG
MX = MW + NREG
MY = MX + NREG
MA1 = MY + NMGEG
MAZ = MA1 + NMGEG*9

```

and MZ which must be redefined as

```
MZ = MA2 + NREG - 1.
```

A description of the new parameters used in Subroutine BIPAR are given below:

```

NRGWB      - Number of regions for which the numerical adjoint flux will be
              input.

PSI(K,J,L) - Numerical adjoint flux for direction K and energy group J.
              The parameter L is a number used to identify each set of data.

LABNP(I)   - The ID number of the set of adjoint flux data input for each
              region. The parameter is equal to zero if no adjoint flux was
              input for that region.

BETA(K,J,L) - The exponential transform biasing parameter for direction K
              and energy group J. The parameter L is an ID number to identify
              each set of biasing parameters.

LABNB(I)   - ID number of the set of BETA data to be used with region I.

PL and SI  - Parameters used in the least squares calculations.

NMGEG      - Number of energy groups plus one for which the adjoint flux
              PSI is input.

EFMGS(I)   - Upper bound of first energy group and the lower bound of each
              successive group.

INPT (I)   - = 1 If the adjoint flux is input for region I.
              = 2 If the adjoint flux is not input for region I.

```

The INPT data for each region should be read from the region description card that is also read for each region in subroutine GEOMIN. The INPUT parameter should be read as the second entry of the card. This location is not presently used.

Appendix

Note that the coordinates of a point within each region that are read in subroutine GEOMIN of COHORT are also used in subroutine BIPAR. In BIPAR, each point is assumed to be near the geometric center of each region. This must be considered when describing the coordinates of the point within the regions in which importance sampling is desired.

The output of subroutine BIPAR is the parameter $BETA(K,J,L)$ which is stored in $S(MT)$. This parameter describes the necessary exponential transformation information for each energy group, region, and direction. These terms correspond to the parameter $B(E',R',N)$ in Equation (3.28). They should be applied in the particle track length selection in H01 using Equation (3.28). The required input into the subroutine is defined in the argument of the SUBROUTINE statement listed in Appendix A.

The subroutines listed in Appendix B were written to calculate the biased scattering distribution, Equation (3.25) and then to sample outgoing gamma-ray energies and directions of motion. There are 8 different subroutines listed. Each of the subroutines is called as needed from subroutine CASK, which is called from various points within H01. CASK is called first at the start of subroutine HIGENE. At this point, the scattering probabilities from the normal scattering distribution are calculated as given by Equation (3.27). The CALL statement for this point should have the format:

```
CALL CASK (1, NRGWB, NMGEG, EFMGS, S(MR), S(MU), S(MA1)) .
```

CASK is called again in subroutine SCATR after the type of interaction has been determined (i.e., Compton scattering or pair production). Note that CASK is not called if importance sampling is not desired in the region in which the collision occurred. The CALL statement should have the format:

```
CALL CASK (LBC, NRGWB, NMGEG, EFMGS, S(MR), S(MU), S(MA1)).
```

The value of LBC must be set in subroutine SCATR according to the following conditions:

- 1) LBC = 0 if no importance sampling is desired
- 2) LBC = 2 for a Compton scattering event if importance sampling is desired and the previous collision occurred in a region in which importance sampling was used.
- 3) LBC = 3 for a Compton scattering event if importance sampling is desired and the previous collision did not occur in a region in which importance sampling was used.
- 4) LBC = 4 if the event was a pair production and importance sampling is desired.

Appendix

The output of subroutine CASK is the energy and direction of the particle after scattering. The particle energy is specified by the parameter E. The direction of the gamma is indicated by the direction cosine given by the parameters A, B, and C. After the program returns to subroutine SCATR from CASK, the program should set the various option parameters such as LBC and TAU and continue with the normal flow of subroutine SCATR. Corrections to the particle weight to account for biased scattering are made in CASK. No other weight adjustments, such as for the omission of absorption, are made in CASK.

The use in COHORT of the importance sampling techniques described above required very little knowledge of the transport problem once the representative three-dimensional adjoint has been specified. The biasing techniques may be applied in any problem in which the previous limited method of exponential transformation would be used. The techniques provide a means of importance sampling the scattering angle in addition to extending the exponential transformation to include energy and angle dependence. The only additional required COHORT input is 1) the adjoint flux for each energy, angle, and region, 2) the energy boundaries of the energy groups for which the adjoint flux is specified, and 3) several specification parameters. The additional energy groups should be in multigroup structure. On the other hand, the exponential transformation parameter will be calculated in the COHORT procedure. It may, therefore, be omitted from the program input.

Appendix

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