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SPHERE: A Spherical-Geometry Multimaterial Electron/Photon Monte Carlo Transport Code

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SPHERE: A Spherical-Geometry Multimaterial Electron/Photon Monte Carlo Transport Code

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ABSTRACT

SPHERE provides experimenters and theorists with a method for the routine solution of coupled electron/photon transport through multimaterial configurations possessing spherical symmetry. Emphasis is placed upon operational simplicity without sacrificing the rigor of the model. SPHERE combines condensed-history electron Monte Carlo with conventional single-scattering photon Monte Carlo in order to describe the transport of all generations of particles from several MeV down to 1.0 and 10.0 keV for electrons and photons, respectively. The model is more accurate at the higher energies, with a less rigorous description of the particle cascade at energies where the shell structure of the transport media becomes important. Flexibility of construction permits the user to tailor the model to specific applications and to extend the capabilities of the model to more sophisticated applications through relatively simple update procedures.

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SPHERE: A Spherical-Geometry Multimaterial Electron/Photon Monte Carlo Transport Code

1. Introduction

The early work of M. J. Berger[1] firmly established the method of condensed-history Monte Carlo for the description of electron transport through extended media. Under the sponsorship of the U.S. space program, this work produced the ETRAN Monte Carlo code system[2] for coupled electron/photon transport in homogeneous media. There are now models, based more or less on this approach, that describe the production and transport of the electron/photon cascade in three-dimensional multimaterial geometries over the energy range from a few tens of MeV down to approximately one keV.[3,4] The very generality of these codes militates against their routine employment in the solution of many practical transport problems. This is due primarily to the substantial amount of card input required.

Although most practical transport problems are of a multimaterial nature, full three dimensionality is not so general a requirement. This report documents program SPHERE, the third of a series of transport models, each of which is designed for a specific geometrical class of problems. The first of these, the TIGER code,[5] is a one-dimensional multislab model. The second, the CYLTRAN code,[6] is appropriate to two-dimensional multimaterial geometries having cylindrical symmetry. The model described here is applicable to one-dimensional configurations consisting of multiple concentric spherical shells. An important feature of programs SPHERE, TIGER, and CYLTRAN is the similarity of their input/output. Consequently, once the user has run any one of them, he will be able to run the other two with very little additional effort.

Programs TIGER and CYLTRAN have seen extensive and varied application within Sandia Laboratories. They are also receiving wide external distribution, which should increase substantially with the completion of code conversions currently under way at ORNL that will permit their use on IBM computers. The development of program SPHERE was motivated by requirements of the pulsed electron beam fusion program for the design and analysis of experiments involving spherical target pellets. However, it may also find important application in space shielding work, in the radiation transport from dispersed radioactive sources, and in the study of local effects of particle loading and other inhomogeneities on radiation transport.

As in References 5 and 6, the organization of this report is oriented toward the needs of the user. Section 2 contains all the necessary information for running the code. From a user point of view, the material following Section 2 is not essential; however, familiarity with it is strongly recommended for a better appreciation of code capabilities. Section 3 is concerned with theoretical verification (data appropriate for experimental verification does not exist) through comparison of the predictions of the SPHERE code with the corresponding results of SANDYL and TIGER calculations. A brief description of the construction of the SPHERE code is given in Section 4. Section 5 contains a review of some of the expanded capabilities that are available through standard update procedures.

Comments and suggestions and/or consultation on any difficulties that may arise in the application of this code are welcomed by the author.

2. Operation

2.1 Control Deck

Experience with TIGER and CYLTRAN has shown that users frequently take advantage of update capabilities such as those described in Section 5. Therefore, the FORTRAN program in update format has been placed on magnetic tape. Figure 1 shows the control deck for running program SPHERE from this file (tape #10855) on the CDC-7600 system. The Small Core Memory (SCM) requirement is 141000 (octal), and the Large Core Memory (LCM) requirement is 245000 (octal). The SCM and LCM requirements are determined by subprograms DATPAC and SPHERES, respectively (see Section 4). Although the program itself is compatible with the CDC-6600 system, the magnetic tape must be rewritten for compatibility with that system.

2.2 Problem Geometry

The problem geometry of program SPHERE consists of a series of concentric spherical shells, which may be either voids or homogeneous material media. The sphere defined by the outer radius of the outermost shell is referred to as the problem sphere. The entire volume within the problem sphere, including the innermost spherical region, must be specified in terms either of material or of void shells. All particles (electrons or photons) that exit the problem sphere are tallied as escape particles. Particle histories are initiated at the surface of the problem sphere (see Section 5.1 for alternative source configurations).

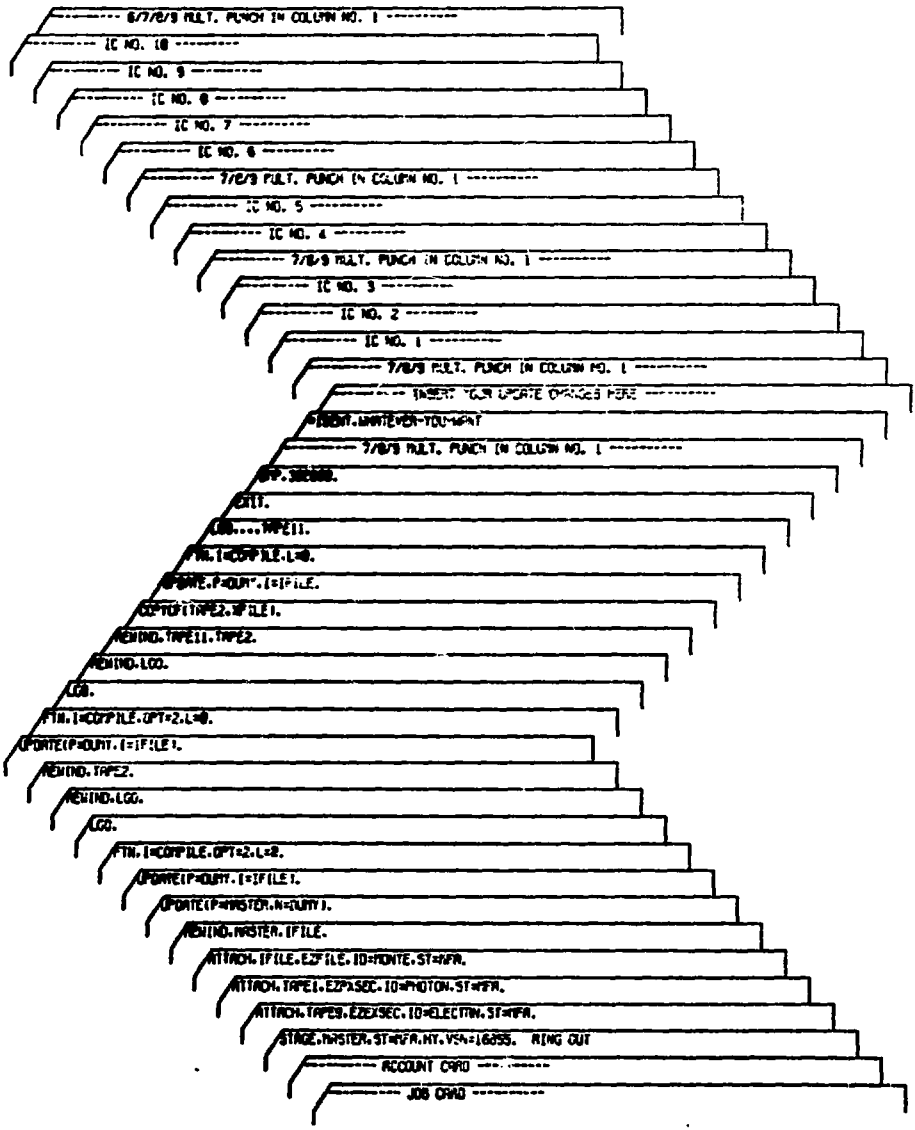

Figure 1. Control deck for running SPHERE from permanent file.

2.3 Input

The similarity of the SPHERE code to the TIGER code derives from the fact that it is strictly one-dimensional in the sense that material geometry, trajectories, and source description are all one-dimensional. Consequently, many of the axial variables of TIGER become radial variables in SPHERE. Table I lists the card input variables required for each card and the formats under which they are read. This input is virtually identical with that of the TIGER code, the only difference being that NLAY, the number of planar zones in the TIGER input, is replaced by NSHL, the number of concentric shells in the SPHERE input.

BLE I

Input Variables and Formats

IC NO.	Variables	Format
1	NMAT, NSET	(12I6)
2[a]	NE	(I5)
3[a]	(IZ(J), W(J), J=1, NE)	(5(I5,E10.0))[b]
4	COMMENT	(18A4)
5[a]	ISTATE, EMAX, RHO, ETA	(I5,3F12.5)
6	INC, JMAX, JPMAX, KMAX, KPMAX, IMAX, NSHL	(12I6)
7	(MAT(I), I=1, NSHL)	(12I6)[b]
8	(NZONE(I), I=1, NSHL)	(12I6)[b]
9	(THIK(I), I=1, NSHL)	(6F12.5)[b]
10	TIN, TCUT, TPCUT, CTHIN	(6F12.5)
11[c]	JSPEC	(I6,66H)
12[c]	(SPECIN(J), J=1, JSPEC)	(6F12.5)[b]
13[c]	(ESP(J), J=1, JSPEC)	(6F12.5)[b]

[a]The pair of ICs, #2 and #3, and IC #5 are to be repeated NMAT times. The order of the repeated pair, #2 and #3, must correspond to that of the repeated IC #5.

[b]Use additional cards if necessary.

[c]Required only for nonmonoenergetic source (see Section 2.4).

The variables listed in Table 1 are defined as follows:

NMAT: Number of unique materials, excluding voids, required in the problem: (≤ 5).

NSET: Arbitrary set number assigned by the user to be used for identification of the run.

(The two cards containing the next three variables must be repeated NMAT times. The order in which the pairs of the cards are read defines the material numbers required on IC #7).

NE: Number of elements in the homogeneous target material: (≤ 10).

IZ: Array of atomic numbers of constituent elements read in ascending order.

W: Weight fraction array corresponding to the IZ-array.

COMMENT: A 72-character comment describing the run.

(The card containing the next four variables must be repeated NMAT times in the same order as the pairs IC #2 and IC #3.)

ISTATE: 1 for a solid or liquid; 2 for a gaseous target material.

EMAX: Incident energy (MeV) for monoenergetic source (electrons or photons) or maximum energy in the case of a source spectrum.

RHO: NTP (0°C, 1 atm) density of the target material (g/cm^3).

ETA: Ratio of actual density to the NTP density of the target material. If left blank (zero), ETA is automatically set to 1.0.

INC: 1 for incident electrons; 2 for incident photons.

JMAX: Number of equal energy bins for classifying escaping electrons (≤ 50).

JPMAX: Number of equal energy bins for classifying escaping photons (≤ 50).

KMAX: Number of equal angular bins for classifying the escaping electrons according to their obliquity with respect to the normal to the sphere at the point of escape (< 18).

KPMAX: Number of equal angular bins for classifying the escaping photons according to their obliquity with respect to the normal to the sphere at the point of escape (≤ 18).

IMAX: Number of histories of primary particles (electrons or photons) to be followed.

NSHL: Number of distinct homogeneous material shells or voids in the problem, including the innermost spherical region (≤ 50).

MAT: Array of numbers identifying the material in each shell of the target, beginning with the innermost shell (sphere). Material number is determined by the order in which the IC #2 and IC #3 pair is read. Zero defines a void shell.

NZONE: Array of numbers specifying the number of zones into which each shell is to be divided for purposes of scoring energy and charge deposition, beginning with the innermost shell (sphere). Total number of zones in the target must be ≤ 50.

THIK: Array of numbers specifying the thickness of each shell, in centimeters, beginning with the innermost shell (sphere).

TIN: Equals EMAX for monoenergetic source, minus EMAX for a nonmonoenergetic source.

TCUT: Cut-off energy (MeV) at which electron histories are terminated. A final adjustment pertaining to the calculation of energy and charge deposition is made (≥ EMAX/244 or 0.001 MeV, whichever is the larger).

TPCUT: Cut-off energy (MeV) at which photon histories are terminated. Upon termination the residual energy of the photon is assumed to be deposited on the spot (≥ 0.010 MeV).

CTHIN: When ≤ 1.0, CTHIN is the cosine of the angle of incidence with respect to the normal to the sphere at the point of entry; for a 2π isotropic source, 1.5; and for a 2π cosine law source, 2.5.

JSPEC:* One plus the number of energy bins in the spectrum (i.e., the number of energy values) of the incident radiation (≤ 31).

SPECIN:* Cumulative probability distribution for the spectrum of incident radiation in descending order. SPECIN (1) must equal 1.0 and SPECIN (JSPEC) must equal 0.0.

ESP:* Energy list corresponding to SPECIN. ESP(JSPEC) ≥ TCUT(TPCUT in the case of a photon source).

*JSPEC, SPECIN, and ESP are read in only when TIN is negative.

2.4 Sample Input for Monoenergetic Source

Figure 2 shows the input data for a problem involving a monoenergetic source. The energy of the radially incident electrons is 1.0 MeV. The geometrical configuration consists of three concentric material shells surrounding a central void that has a radius of 10.0 cm. This is the input data used to obtain the energy and charge deposition profiles in Figures 5 and 6, as described in Section 3.

2.5 Sample Input for a Source Spectrum

Figure 3 shows the input data for a nonmonoenergetic (1.0-MeV, maximum) source that is radially incident upon the same material configuration as was described in the previous subsection. The only changes relative to Figure 2 are

a. The problem title has been changed.

b. TIN has been changed from 1.0 to -1.0.

c. The additional cards describing the spectrum (IC #11, IC #12, and IC #13) have been added immediately after IC #10.

The source energies will be sampled from the spectrum shown in Figure 4. Note that only that portion of the spectrum above TCUT is employed in determining the cumulative distribution. For example, SPECIN (3), which is the fractional number of source electrons below 0.6 MeV but above TCUT (0.1 MeV), is given by

$$\text{SPECIN (3)} = \frac{5\% + 15\% + 25\%}{5\% + 15\% + 25\% + 35\% + 30\%} = 0.45 \quad .$$

2.6 Suggestions for Efficient Operation

Operational limitations on input variables are given in Section 2.3. Physical limitations are discussed by the authors in Reference 2. Here we wish only to point out that the choice of certain input parameters can markedly affect the efficiency of the calculation; that is, the user's ability to obtain statistically meaningful output in a reasonable amount of time.

a. Obviously, the number of histories, IMAX, should be kept as small as possible. The SPHERE code provides the user with estimates of the statistical accuracy of the output data.* This information serves as a guide in the choice of IMAX.

*See 2.7 for further details.

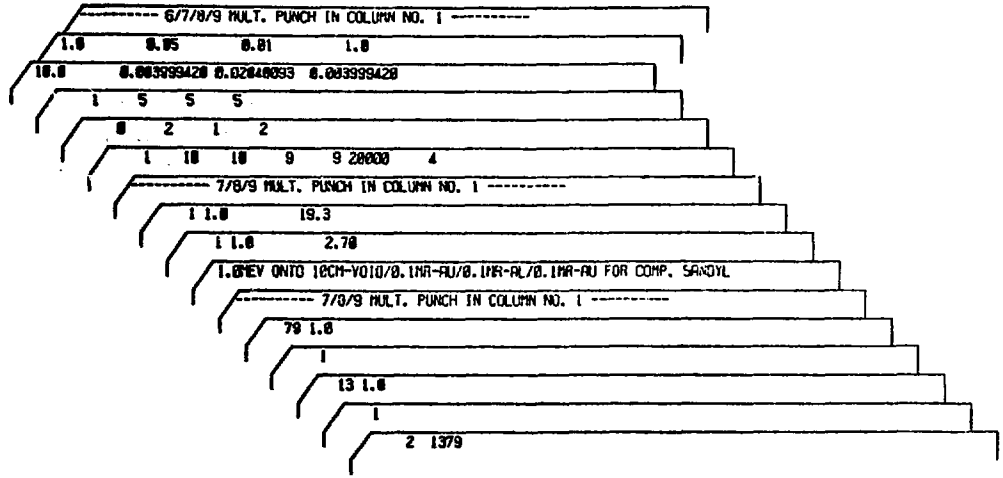

Figure 2. Sample input for running a problem with a monoenergetic source.

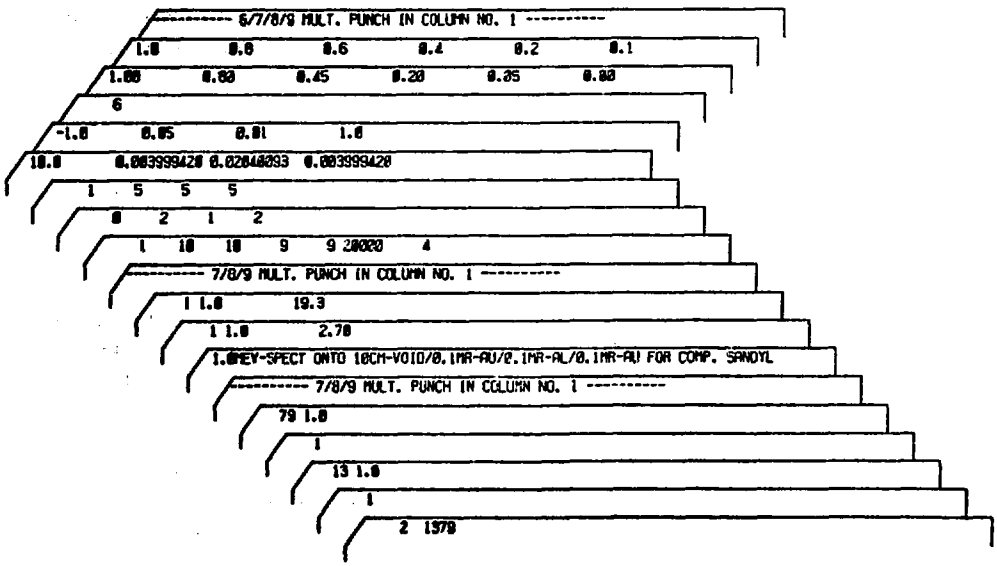

Figure 3. Sample input for running a problem with a nonmonoenergetic source.

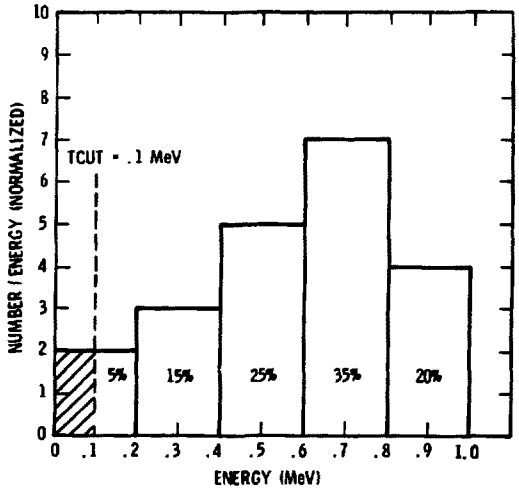

Figure 4. Source electron spectrum from which the cumulative probability distribution listed in Figure 3 was obtained.

b. TCUT should be as large as possible. For example, if the source is monoenergetic, TCUT equal to 5 or 10 percent of TIN should be adequate. Because the logarithmic energy grid used in this technique becomes much finer at low energies, following histories down to low energies becomes very time consuming. On the other hand, running time is not very sensitive to the value of TPCUT.

c. JMAX, JPMAX, KMAX, KPMAX and the number of deposition zones should be as small as possible. Demanding excessive energy, angle, or spatial resolution only makes it more difficult to obtain statistically meaningful output.

2.7 Output

In addition to certain diagnostic information the basic output consists of

a. Energy and number escape coefficients for both electrons and photons.

b. Charge and energy deposition profiles.

c. Escape coefficients that are differential in energy for both photons and electrons.

d. Escape coefficients that are differential in angle for both photons and electrons.

e. Coupled energy and angular distributions of escaping photons and electrons.

Every output quantity is followed by a one- or two-digit integer that is an estimate of the 1-sigma statistical uncertainty of that quantity expressed in percent. Details of the method used to obtain these statistical data are given in Section 4.5L.

3. Verification

There are no experimental results which can be compared with the predictions of program SPHERE. Of the existing codes capable of describing electron/photon transport in concentric spherical shell configurations, the physical data and numerical procedures of the three-dimensional SANDYL code most closely approximate those of the SPHERE code. In this section we will compare the predictions of SANDYL and SPHERE for a three-shell configuration. Letting the radius of the central void become very large and letting this void also absorb particles (through a temporary update), the results of the SPHERE code are also compared with those of the TIGER code.

3.1 Comparison With SANDYL

In the problem chosen for the SANDYL comparison, 1.0-MeV electrons are radially incident upon a configuration consisting of a 10.0-cm-radius central void surrounded by three concentric material shells. The middle shell is Al with a thickness of 0.1 times the CSDA range of the source electrons. It is sandwiched between two Au shells, both of which also have thicknesses of 0.1 times the CSDA range. The card input data for this problem is shown in Figure 2. The energy deposition profiles predicted by the SANDYL and SPHERE codes are compared in Figure 5. Although the agreement is good, the differences at large depths are greater than the 1-sigma statistical uncertainties (about 1 percent). The same general comments hold for the comparison of charge deposition profiles in Figure 6, except that the statistical uncertainties are of the order of 5 percent. Table II is a comparison of the integral escape coefficients. Again the disagreement in electron coefficients is slightly greater than the 1-sigma uncertainties. These uncertainties were obtained from the SPHERE calculation and are assumed to hold also for the SANDYL results. Combining the results from Table II with the total absorption from Figure 5 shows that energy conservation in both codes is excellent.

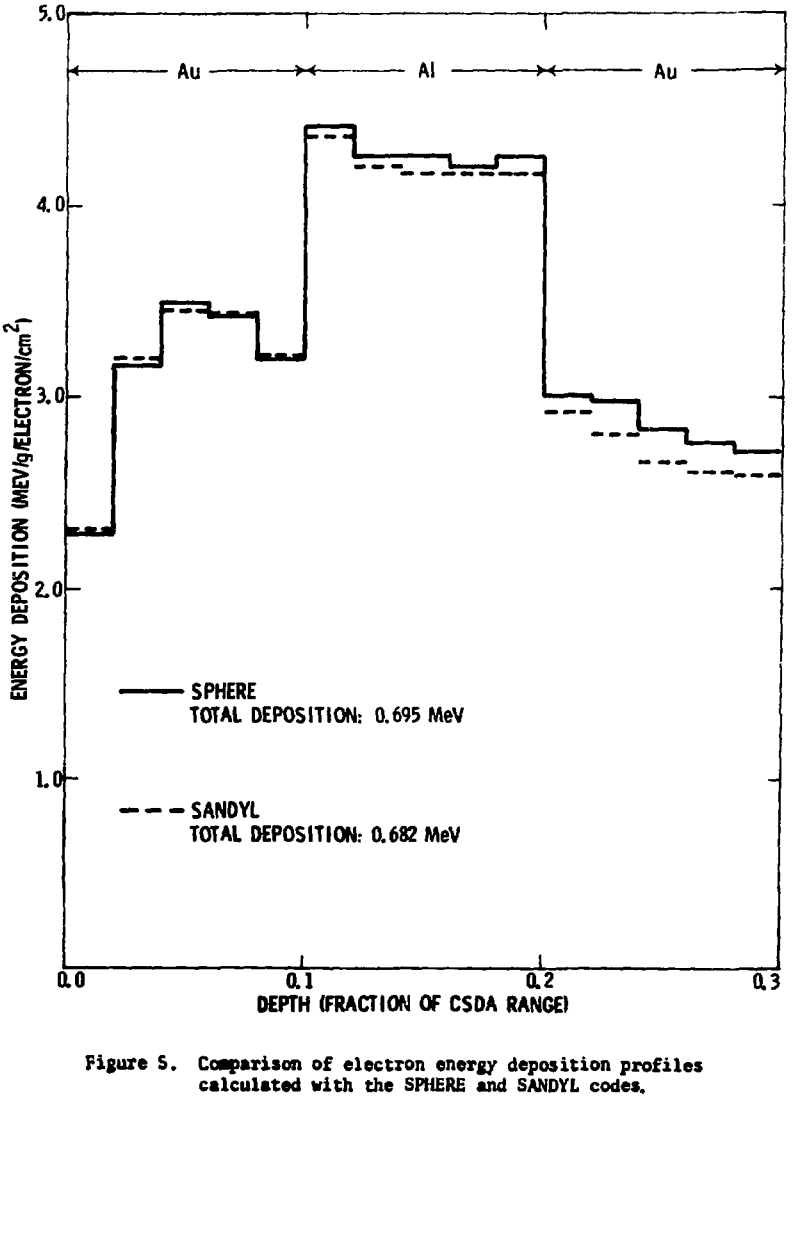

Figure 5. Comparison of electron energy deposition profiles calculated with the SPHERE and SANDYL codes.

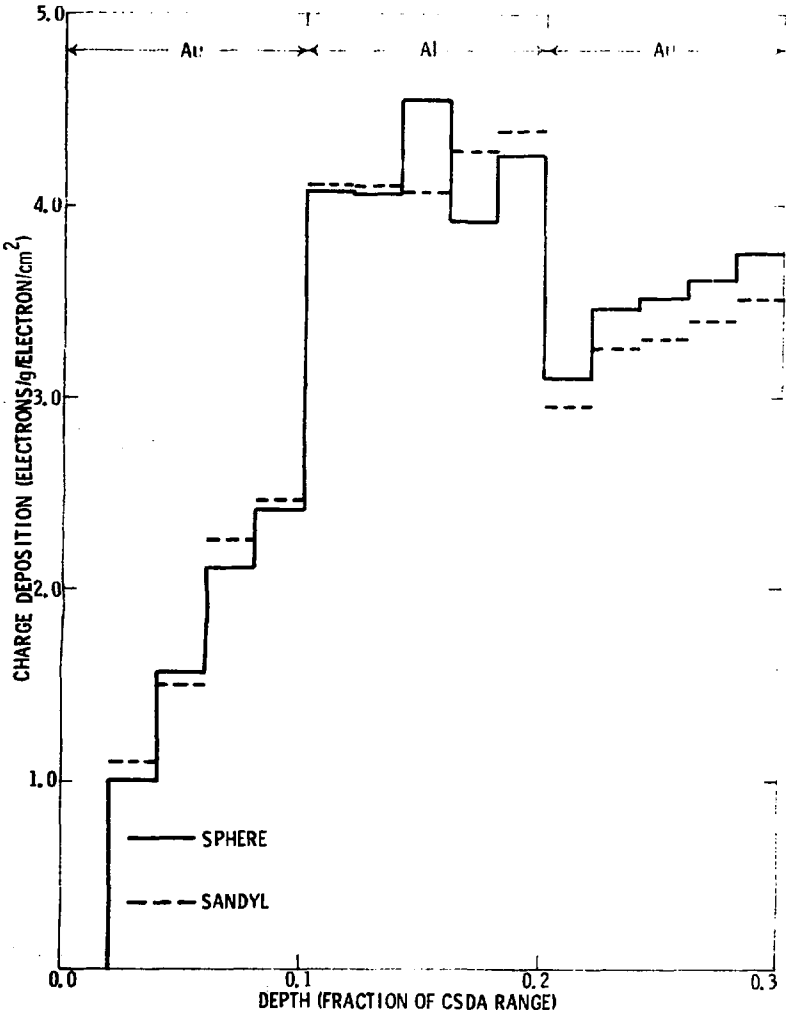

Figure 6. Comparison of electron charge deposition profiles calculated with the SPHERE and SANDYL codes.

TABLE II

Comparison of Integral Escape Coefficients Obtained From the SANDYL and SPHERE Codes. The statistical uncertainty is expressed as a percent of the given coefficient.

Type	Coefficient (%)		Statistical Uncertainty (%)
	SANDYL	SPHERE	
Electron Number	41.0	39.1	1
Electron Energy	29.7	28.4	1
Photon Number	12.0	11.6	2
Photon Energy	2.16	2.10	4

3.2 Comparison With TIGER

The cross-section data and many of the numerical algorithms of the SPHERE code are identical with those of the TIGER code. Thus, a comparison between TIGER and SPHERE might be considered a better test of the validity of the SPHERE code. The radius of curvature of the central void in the SPHERE calculation of the previous section (10 cm) is already sufficiently large that transmission through the three material shells should be accurately described by a multislab code such as TIGER. However, there was an additional requirement that the central void absorb particles so as to prevent their crossing the void and reentering the material. This was accomplished through a temporary update.

Comparisons of the energy and charge deposition profiles are shown in Figures 7 and 8, respectively. The integral escape coefficients of the SPHERE code are compared with the integral reflection coefficients of TIGER in Table III. Agreement between the two codes is excellent.

Since the TIGER and SPHERE codes were developed by the same authors, and the SANDYL and SPHERE codes were not, the small disagreement between the SANDYL and SPHERE predictions is probably due to a combination of subtle differences, both in the physical assumptions and in the numerical algorithms.

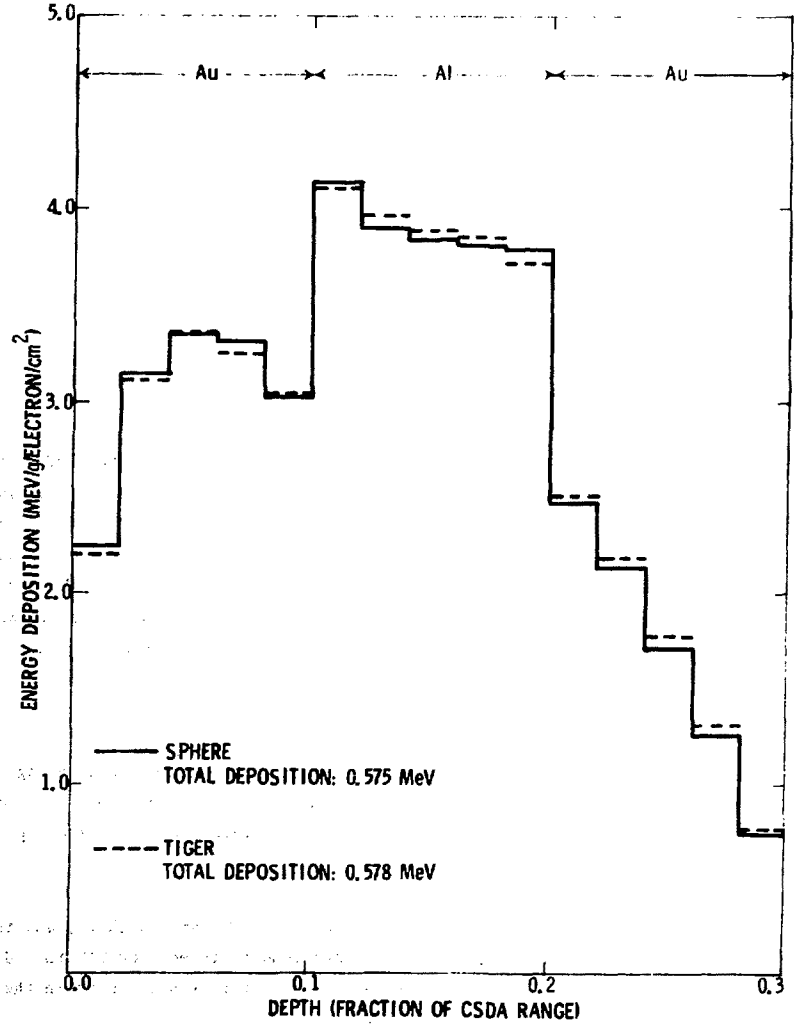

Figure 7. Comparison of electron energy deposition profiles calculated with the SPHERE and TIGER codes.

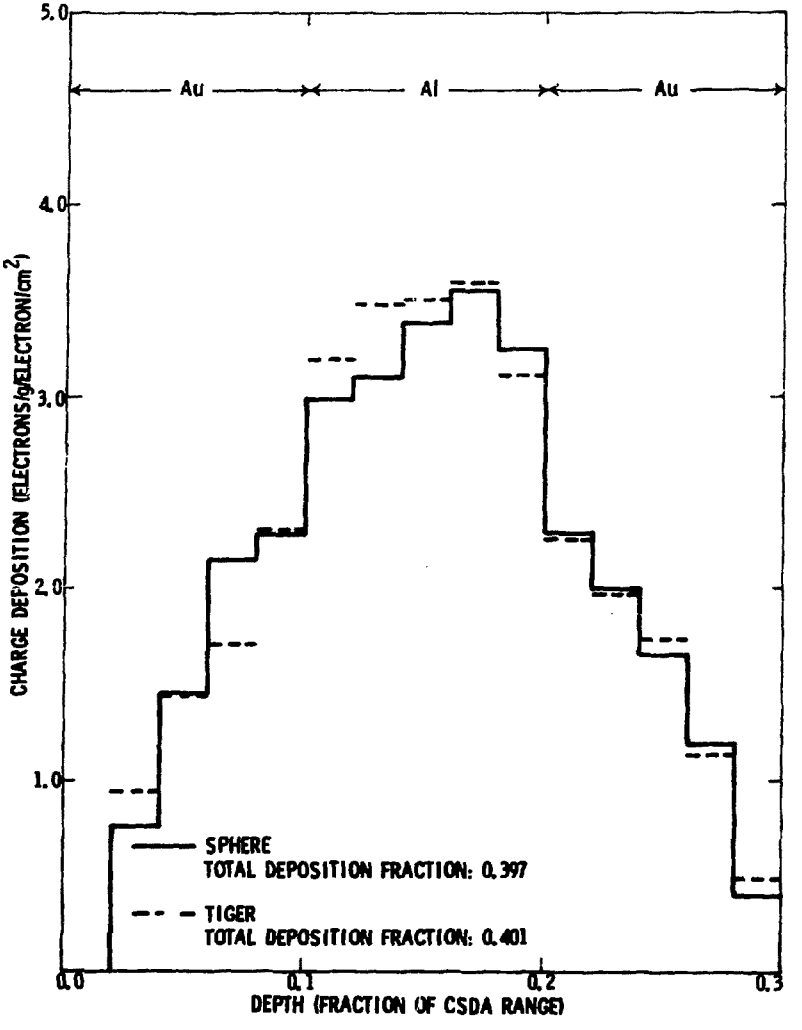

Figure 8. Comparison of electron charge deposition profiles calculated with the SPHERE and TIGER codes.

TABLE III

Comparison of the Integral Reflection Coefficients Obtained From the TIGER Code With the Integral Escape Coefficients Obtained From the SPHERE Code. The statistical uncertainty is expressed as a percent of the given coefficient.

Type	TIGER Reflection Coefficient (%)	SPHERE Escape Coefficient (%)
Electron Number	38.3 ± 1	39.4 ± 1
Electron Energy	27.9 ± 1	28.7 ± 1
Photon Number	5.53 ± 3	5.41 ± 2
Photon Energy	0.848 ± 4	0.808 ± 3

4. Construction

The SPHERE code consists of two BCD permanent files, EZPXSEC and EZEXSEC, and a magnetic tape file in update format which contains three subprograms. The two BCD files and the first two subprograms, which are used for cross-section generation, are also components of the TIGER[5] and CYLTRAN[6] codes.

4.1 EZPXSEC

EZPXSEC, the photon-cross-section library, is essentially the cross-section data of Biggs and Lighthill[7,8] in modified format and is identical with the photon library used in the TIGER and CYLTRAN codes.

4.2 EZEXSEC

EZEXSEC, the electron-cross-section library, was constructed by Berger and Seltzer and is referred to in their ETRAN Monte Carlo code system[3] as LIBRARY TAPE 2. It is distinguished from other library tapes of the ETRAN system in that the empirical corrections to the bremsstrahlung cross sections are based upon the experimental data of Rester[9] and Aiginger.[10] This same cross-section library is employed in the TIGER and CYLTRAN codes.

4.3 PGEN

PGEN is the first of three subprograms in update format which make up the magnetic tape file. Using the file EZPXSEC and the data from IC #1, IC #2 and IC #3 of Table I, it prepares the photon sampling distributions required by the Monte Carlo subprogram. These distributions cover an energy range from 1000 MeV down to 10 keV. This subprogram is identical with the corresponding subprogram of the TIGER and CYLTRAN codes. It uses the data of Wapstra[11] for the average K-fluorescence energies. Again, fluorescence and Auger production are allowed for only the highest-Z element of each material, regardless of its weight fraction.

4.4 DATPAC

This second subprogram of the magnetic-tape file prepares the electron sampling distributions for the Monte Carlo subprogram. Using the EZEXSEC file, IC #5, and material data transferred from subprogram PGEN, it generates the same distributions as does the identical subprogram of the TIGER and CYLTRAN codes.

4.5 SPHERES

SPHERES is the last of the three subprograms that make up the magnetic tape file. The construction of SPHERES constituted most of the effort in the development of the SPHERE code. SPHERES is a hybrid of the corresponding subprograms of the TIGER and CYLTRAN codes. The following discussion of the more important features of this subprogram emphasizes comparisons with existing multimaterial codes.

A. Trajectories -- Trajectories in the SPHERE code are strictly one-dimensional. The origin of the coordinate system is the center of the problem sphere. Particle location is defined by the length of the radius vector to its position. Particle direction is defined by the direction cosine of its velocity with respect to this radius vector. There is a great deal of similarity between the trajectory logic of the SPHERE code and that of the one-dimensional TIGER code. In the SPHERE code, however, the vector analytic geometry of the trajectories is complicated by the spatial dependence of the direction cosine along a rectilinear random walk substep.

B. Zoning -- Specification of shell boundaries and subzoning within a given homogeneous material shell is also quite similar to layer specification and subzoning in the TIGER code. On the other hand, a capability for including void zones becomes necessary in spherical geometry. The additional logic required to accommodate void

zones is considerable. This additional logic is avoided in some codes[5] by simulating voids with very low density gases. We believe allowance for actual voids to be preferable for three reasons. First, a faster code should result because void transport bypasses many collisional algorithms. Second, a more accurate code should result because void transport is rigorous, whereas condensed-history electron transport through small-areal-density simulated voids involves a number of approximations. Finally, a substantial amount of additional memory is required for the cross-section data of the simulation gas (see Section 4.5F).

C. Boundary Crossings -- Photon transport in SPHERES is accomplished via conventional microscopic Monte Carlo methods,[12] where particle trajectories that cross material boundaries pose no unusual problems. On the other hand, when the condensed-history Monte Carlo substep of an electron crosses a material boundary, certain approximations must be invoked. The procedures employed in the SPHERE code are equivalent to those used in the TIGER code and are discussed in Section 4.5B of Reference 5.

D. Shell Effects -- The treatment of ionization and relaxation effects within the stopping media is not nearly so detailed in the SPHERL code as it is in SANDYL. Photoionization and electron impact ionization, as well as subsequent relaxation via fluorescent and Auger processes, are considered only in the case of the K-shell of the highest-atomic-number element of a given material. Photon transport below 10 keV is not allowed. Thus, for those applications in which shell ionization and relaxation effects are expected to have a significant effect upon the output of interest, the SANDYL code is to be preferred over the SPHERE code.

E. Statistics -- Under the normal default option, the IMAX histories are run in 10 equal batches. The output routine is called at the end of each batch. Immediately before each write statement, a call is made to subroutine STATS. This routine recalls the statistical variables corresponding to the output quantities about to be written, computes the estimate of the standard error--in percent--based on the number of batches that have been run, and transfers the statistical parameters required for the subsequent batch back to Extended-Core Storage (ECS) (LCM on CDC-7600). Unless modified by update, only the final results based on the total number of completed batches are printed out. The user may specify a number of batches other than 10 by inserting the desired number in field 8 of IC #6.

A corollary of batch processing is a feature that prevents the user from exceeding his time limit. Before beginning a new batch, the remaining portion of the time requested for the job is compared with an estimate of the time per batch. If this

estimate is larger than the time remaining, results based on the number of completed batches--including estimates of the statistical errors--are printed out and the run is terminated.

Under normal operation, virtually every Monte Carlo output quantity is followed by a one- or two-digit integer from 0 through 99 (estimates even greater than 99 are shown as 99) that is the best estimate of the statistical standard error expressed as a percent of the final value:

$$(S.E.)_N = \frac{100}{|\langle x_N \rangle|} \left\{ \left| \frac{\langle x_N^2 \rangle - \langle x_N \rangle^2}{N - 1} \right| \right\}^{1/2} ,$$

where

$$\langle x_N \rangle = \frac{1}{N} \sum_{i=1}^{N} X_i ,$$

and

$$\langle x_N^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} X_i^2 .$$

The X_i's are the values of the quantity obtained from each batch, and N is the total number of completed batches (usually 10).

F. Core Requirement -- Core requirement was an important consideration in the construction of the SPHERE code. About 15600 (decimal) variables are required for each material. Merely adding a material index to these variables would severely limit the number of materials allowed in a calculation. Furthermore, a large core requirement generally lowers job priority and increases turnaround time. The approach taken in SANDYL was to reduce the resolution of the larger distributions and to replace the largest, the bremsstrahlung energy and angular distribution, by a simple analytic formula. This approach was avoided in the construction of SPHERES by making use of the capability for Extended-Core Storage (ECS) available with the local CDC-6600 system (LCM on CDC-7600 system).

By putting the three largest electron-cross-section arrays in ECS (LCM) and recalling them into central memory (SCM on CDC-7600) only when needed, the requirement for a material index for about 10000 of the above 15600 variables was avoided. Thus, only 10000 locations of Central Memory (SCM) are required for these three arrays, regardless of the number of materials in the problem configuration. Two large photon-cross-section arrays, accounting for about 2700 of the 15600 variables, are also stored in ECS (LCM). These photon-cross-section variables are recalled individually, rather than by the entire array; thus, no central memory at all is required for these 2700 variables.* Since the remaining variables are arbitrarily dimensioned for five materials, the total ECS (LCM) requirement for cross-section data is about 63500 (5 x 12700) decimal locations.

An additional ECS (LCM) requirement of 20400 decimal locations for statistical variables leads to a total ECS (LCM) requirement of approximately 245000 octal locations.

5. Updates

In the development of the SPHERE code, our primary motivation was to provide scientists and engineers with a method characterized both by theoretical rigor and by operational simplicity for routine solution of multimaterial problems having spherical symmetry. The rigor was achieved through the internal selection of the most general options. Operational simplicity is the keynote of Section 2. However, the deterministic nature of the Monte Carlo procedure, the completness with which the SPHERE code describes the radiation transport, and the flexibility of construction make it possible for the user to significantly extend the capabilities of the code with relatively simple updates. In this section several updates that the authors have found useful are reviewed in varying degrees of detail. The list is by no means exhaustive, and users are encouraged to consult with the authors concerning specific applications.

5.1 Source Routines

The standard source (according to which particle histories are initiated at the surface of the problem sphere and according to which energy and angular distributions are selected by the parameters TIN and CTHIN) should be adequate for most applications.

---

*If this same procedure is used to eliminate the 27000 decimal locations required for the W1-array of the SANDYL code, about 65000 octal locations of Central Memory will be released. Furthermore, since the indexing arithmetic is already present in SANDYL, the increase in running time might be negligible.

Consequently, we have chosen not to overwhelm the user with a myriad of source options. The resulting simplicity and flexibility in the coding of the source routine make it easy for the user to construct a source of arbitrary spatial, energy, and angular distribution. The user need only modify that portion of Subroutine HIST between statements 10 and 50 to fit his particular application.

The only essential restriction is that all source positions must lie within the problem sphere; for example, in the standard source routine the code internally shifts the radial coordinate 10^{-7} cm inside the surface of the problem sphere to ensure that this restriction is satisfied.

5.2 Multiple Problems

The user may obtain the results for an arbitrary number of problems in a single run with the update

```
*DELETE,EZTRN.228
     IRNMAX = "desired value."
```

ICs #1 through #5 are not repeated; they must contain sufficient information for the production of all electron and photon cross sections required for the multiple Monte Carlo calculations. The group of ICs beginning with #6 must be repeated for each problem. This update is especially useful in parameter studies. Although its use will prevent multiple turnaround time and repetition of cross-section calculations, it must be remembered that a multiple problem run necessarily requires more machine time.

5.3 Scaling of Bremsstrahlung Production

This update is especially useful in bremsstrahlung converter studies. With the update

```
*INSERT,TIGER.146
     BNUM(1) = "desired value,"
```

the user may artificially increase the bremsstrahlung production to improve the statistical accuracy of bremsstrahlung output without increasing the number of primary electron histories, which would be much more time consuming. The cross sections of material #1 are scaled so that an electron slowing-down from TIN to TCUT in this material will, on the average, generate BNUM(1) bremsstrahlung photons. The resulting

scale factor is used to scale the bremsstrahlung cross sections for all other materials in the problem. Material #1 should be that material which one would expect to dominate the bremsstrahlung production. Simultaneous scaling of the K-ionization probability may be desirable (see Section 5.4).

This update is used primarily for the prediction of external bremsstrahlung production (e.g., prediction of the environment of x-ray sources). Consequently, a Russian Roulette procedure is employed to reduce the number of secondary electrons generated from the interaction of this artificially high bremsstrahlung population to the naturally occurring number. Although this procedure is very efficient for predicting external bremsstrahlung, it leads to statistically poor and sometimes misleading results for bremsstrahlung deposition. In the latter case, the additional update

```
*INSERT,TIGER.225
     DELIM(1) = 1.0
```

will ensure that all secondary electrons are followed.

5.4 Scaling of K-Ionization Probability

An update option similar to that of the previous subsection permits the user to artificially increase characteristic x-ray production by scaling the cross section for electron impact ionization of the K-shell of the highest-atomic-number element in each material. With the update

```
*DELETE,EZTRN.262
     XNUM = "desired value,"
```

the K-ionization cross section of each material is scaled so that an electron slowing-down in that material from TIN to TCUT will, on the average, generate XNUM K-ionization events.

5.5 TSAVE

In certain problems where only electrons that cross certain boundaries are important, the variable TSAVE may be employed through update to reduce running time significantly. Under normal operation TSAVE is internally set equal to TCUT, but it may be set equal to any value greater than TCUT through update. It becomes operational when an electron is trapped; that is, does not have enough energy to escape from a zone. When an electron with energy greater than TCUT but less than TSAVE is trapped,

it is immediately terminated by the same method as for electrons whose energy falls below TCUT. This parameter is commonly used when one is primarily interested in those electrons escaping from the problem sphere. In this case the update is simply

```
*INSERT,EZTRN.295
    TSAVE = "desired value."
```

Great care should be taken in employing this update where bremsstrahlung production or effects may be important, since bremsstrahlung production is not allowed during terminal processing.

5.6 Forced Photon Collisions

Through update, the user may force photons to interact in certain regions where their natural interaction probability would make it difficult to obtain statistically significant results. The update is

```
*INSERT,ETRANS.906
    PTCZ ("desired zone index") = "desired value for that zone."
```

For example, if PTCZ(6) = .55, then any photon in Zone 6 will have a 55-percent probability of interacting before leaving that zone. The user may force interactions in as many zones as he desires, and the forced interaction probability may be less than, as well as greater than, the natural probability.

5.7 Substep Size

DRANGE/ISUB (see DATPAC-4 output) is the substep size in g/cm^2. When not updated, ISUB is generated internally as a function of material atomic number. For very small zones substep size may be comparable to the dimensions of certain shell thicknesses. This can lead to inaccuracies in condensed-history Monte Carlo. It is suggested that the chosen value of ISUB be sufficiently large that the maximum value of DRANGE/ISUB is no larger than one-tenth of the thickness of any shell of that material. The update is

```
*INSERT,EZTRN.80
    IF (NRUN .EQ. "desired value") ISUB = "desired value."
```

5.8 To Change the Number of Allowed Deposition Zones

To change the number of allowed deposition zones, the user simply redimensions the appropriate variables in common blocks OUT and PUNK (see subroutine OUTPUT of

the SPHERE code listing). The appropriate variables in common block Off have been grouped together to facilitate this update.

5.9 Miscellaneous

Other updates that may be useful in various applications are

a. Extension of photon transport down to 1.0 keV.

b. Calculation of the spectrum of the internal electron flux.

c. Spectrum of absorbed energy within a given zone; that is, the pulse height distribution for that zone without experimental distortions.

d. Selected punched-card output.

e. Intermediate batch output.

f. Changing the starting random number.

The forms of some of these updates depend upon the particular application.

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