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MONTE CARLO MODELING AND FORTRAN
SIMULATION OF A COMPTON BACK-
SCATTER THICKNESS GAGE

C. M. Davenport

UNION CARBIDE CORPORATION
NUCLEAR DIVISION
OAK RIDGE Y-12 PLANT

operated for the ATOMIC ENERGY COMMISSION under U. S. GOVERNMENT Contract W-7405 eng 26

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**MONTE CARLO MODELING AND FORTRAN SIMULATION
OF A COMPTON BACKSCATTER THICKNESS GAGE**

C. M. Davenport

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ABSTRACT

The Monte Carlo technique has been used to create a mathematical model of a class of coating-thickness gages based on Compton backscatter. Disc or point sources of gamma radiation are exposed to a coated target through conical-beam geometry. First-order Compton backscatter is picked up by a disc-shaped detector with a constant-energy response and a conical-beam geometry. Response, in general, is a function of the material properties and thickness of the coating material.

A FORTRAN computer program for efficient simulation of the model has been provided. The more important parameters of the target and detector are variable (individually) during a run; all other parameters and material properties are inputs to the program. Output is in the form of a table and graph of detector response versus any of the variable parameters such as detector orientation and thickness of coating. Provision has been made for easy optimization of the Monte Carlo calculation for any particular problem setup.

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SUMMARY

A computer model has been developed which simulates a Compton backscatter thickness gage. Gamma radiation from the source is Compton scattered in the coating and substrate. Because of a difference in absorption and scattering cross sections between the coating and substrate, the detector response will be a function of the areal density, ρt , of the coating.

The model is based on a Monte Carlo technique which generates at random a representative sample of photon paths from source to detector. The response of the detector is then proportional to the average of the probabilities of successfully executing the individual paths, to an approximation depending on the sampling accuracy.⁽¹⁾ The probabilities are known functions of the material constants. The model considers only Compton scattering and only singly-scattered photons, hence is useful only in the Compton-dominant region, as defined by Evans.⁽²⁾

The FORTRAN IV program is set up to generate a table and graph of detector response as a function of any of the following parameters: α_d , D_d , β_d , A , t , N , or E_ν . In addition, a table and graph of execution time versus the value of an optimizing parameter for the Monte Carlo calculation may be obtained. This feature is useful for optimizing the calculation when a series of similar runs is planned. In addition, it can become a diagnostic tool for estimating running times and locating the source of trouble if a calculation breaks down. For any of the detector response runs, a maximum execution time may be set; at the end of this time, the results thus far calculated are printed out normally.

A comparison with experiment was made for the case of response versus coating thickness. Steel was used as the coating and aluminum as the substrate. Gamma from a gadolinium source, having an energy of 100 kev, were scattered through a relatively well-collimated geometry. The scattered gammas were detected by a thallium-activated sodium iodide crystal. The model agreed with experiment to within a few percent over a range of steel thickness from zero to 240 mils. All qualitative aspects of the curve shape were reproduced.

INTRODUCTION

A very common problem encountered in nondestructive testing and radiation shielding work is the problem of measuring the amount or thickness of a coating on some substrate. It is sometimes feasible to establish a density-times-thickness (DXT) gage on gamma backscatter if the coating absorbs and reflects the rays with different efficiency than the substrate. A mathematical model of such a gage would be useful for establishing feasibility, simulating behavior, and estimating sensitivity.

The properties of gamma radiation which would be used in the mathematical model are well known,⁽³⁻⁷⁾ and the physical laws governing gamma interactions at a level which applies here are, for the most part, simple and concise, at least on an atomic scale. Most of the problems hindering mathematical modeling come about as a result of the mathematically intractable geometry encountered in almost all problems of interest. For instance, a common backscatter gage would have the "intersecting cone" type of geometry. A first approach might be to consider the source beam and target as continuous quantities and do an integration over the interaction effects in the material. However, the volume of interaction is the intersection of two cones, arbitrarily oriented and displaced. This procedure would require a very painstaking numerical integration in three dimensions and would be impractical.

An alternative method would be to consider the source beam as made up of discrete particles (photons) whose physical laws are understood. The progress of a particular photon into the target and out to the detector is a matter of chance, but the various probabilities along the way are fairly well known.⁽⁸⁻¹⁰⁾ A representative sample of photon histories can be chosen which closely approximate the action of the beam in the material. An individual history is easy to calculate even in the presence of complicated geometry; and, as will be shown later, the beam may be closely represented by a surprisingly small photon sample, if properly chosen. The technique used to select a representative sample is called Monte Carlo selection, after its probabilistic aspects.

The objective of this report is to describe a flexible mathematical model of a gamma backscatter gage of the "intersecting cone" geometrical type, and to present a computer program that simulates most cases of practical interest.

MODEL OF A BACKSCATTER GAGE

THE MONTE CARLO MODEL

If the source beam is considered to be composed of discrete particles, the possibility arises that the behavior of the beam can be represented by a carefully selected small sample. In theory, the infinite number of possible paths can be arranged into a probability distribution which will be a function of the problem parameters. A random sampling technique could be used to select a representative sample of photon paths, and then the appropriate reflection coefficient or detector response could be calculated directly from this sample and the physical interaction laws. The accuracy would be as good as the sampling accuracy.

In practice, it is more efficient to construct probability distributions for individual path parameters, such as a point of origin, target intercept, or depth of penetration, and sample from them sequentially to construct one possible path. Any individual distribution will involve fewer problem parameters. Figures 1 and 2 should be referred to in the discussion that follows which outlines the approach taken in this discussion.

Figure 1. EXPERIMENTAL GEOMETRY FOR THE BACKSCATTER THICKNESS GAGE.
(Both Beam Axes are in a Plane which is Perpendicular to the Coating Surface)

Figure 2. A TYPICAL PHOTON PATH, SHOWING THE VARIOUS DESCRIPTIVE PARAMETERS. (μ_{ij} = Linear Attenuation Coefficients)

Construction of a single photon path begins at the source and is extrapolated forward. First, a source intensity function is used as a probability distribution and a source point is picked at random from this. Next, using the source point as an emission source, a target surface interface intercept is picked at random by assuming a $1/r^2$ intensity variation; that is, target surface points are generated at random from a uniform distribution, the "r" distances are calculated, and then the $1/r^2$ distribution is applied via the rejection⁽¹¹⁾ technique. Now the incident direction and intercept are fixed. Next, a penetration depth is generated at random from the known intensity variation with depth, taking into account the direction in the material. An interaction is assumed to take place at this penetration. Finally, the last segment of the path is fixed by generating at random (from a uniform distribution) detector points and then weighting them with a Klein-Nishina angular distribution and a $1/r^2$ intensity distribution about the interaction point via the rejection technique. If this whole process is repeated enough times to see the effect of the various weightings, a representative sample will be obtained.

Having a single path, the probability that a photon can successfully negotiate it is:

probability of survival = probability of penetrating to depth p ,

X probability of Compton scatter interaction,

X probability of scattering toward target, and

X probability of escaping material.

This expression is mathematically different for penetrations into and through the coating:

$$\text{Prob (coating)} = \left[e^{-\mu_{11}p} \right] \times \left[\frac{\sigma_{s1}}{\sigma_{t1}} \right] \times \left[\frac{d\sigma_s}{\sigma_s} \Big|_{\theta, E_1} \right] \times \left[e^{-\mu_{12}d_{\text{esc}}} \right], \text{ and } (1)$$

$$\begin{aligned} \text{Prob (substrate)} = & \left[e^{-\mu_{11}t/\sin\xi - \mu_{21}(p - t/\sin\xi)} \right] \times \left[\frac{\sigma_{s2}}{\sigma_{t2}} \right] \times \\ & \left[\frac{d\sigma_s}{\sigma_s} \Big|_{\theta, E_1} \right] \times \left[e^{-\mu_{22}d_t - \mu_{12}(d_{\text{esc}} - d_t)} \right], \end{aligned} \quad (2)$$

where:

σ_{si} represents the Compton scattering cross section, and

σ_{ti} the total interaction cross section without coherent scattering.

The probability that a photon will survive along a particular path is just the reflection coefficient for that path. If a representative sample of paths is available, the macroscopic reflection coefficient is just the average of the survival probabilities of the sample. This expression can be written:

$$R = \frac{I}{I_0} = \frac{1}{N} \sum_{i=1}^N \text{prob}_i. \quad (3)$$

There will be two summations, corresponding to separate contributions from the coating and substrate. From Equations 1 and 2, they are:

$$R = \frac{1}{N} \left\{ \left(\frac{\sigma_{s1}}{\sigma_{t1}} \right) \sum_{i=1}^M \left(\frac{d\sigma_s}{\sigma_s} \right)_{\theta_i, E_1} e^{-\left(\mu_{11} p_i - \mu_{12} d_{esc_i} \right)} + \right. \\ \left. \left(\frac{\sigma_{s2}}{\sigma_{t2}} \right) e^{-\left(\mu_{11} - \mu_{21} \right) t / \sin \xi} \sum_{i=1}^{N-M} \left(\frac{d\sigma_s}{\sigma_s} \right)_{\theta_i, E_1} e^{-\left[\mu_{21} p_i - \mu_{22} d_{t_i} - \mu_{12} \left(d_{esc_i} - d_{t_i} \right) \right]} \right\} \quad (4)$$

where M represents the number of paths which show penetration into the coating only, and N the total number of paths in the sample. The detector response is then directly proportional to R . The constant of proportionality must be determined from experiment.

Mathematical derivations for the various path descriptors are given in Appendix A. These derivations along with Equation 4 constitute a mathematical model of the gage.

AN ALGORITHM FOR COMPUTER IMPLEMENTATION

The algorithm developed here generally follows the sequence just described for constructing photon paths to make a representative sample. However, certain steps must be taken to optimize the flow through the sequence. Dead-end calculations must be recognized and compensated for. An example is a situation where a given incident direction nowhere intercepts the detector cone. Construction of the rest of the path cannot proceed, and the computer must be programmed to drop this path and go on to another. In addition, some allowed geometries may cause a very inefficient calculation based on the simple sequence previously described. Provision must be made for running a fixed length of time and then printing out the results to that point, because it is very difficult to estimate running time for all cases. Finally, the usefulness of the program depends upon its having options for calculating response as a function of any of a number of parameters.

A flow chart of the algorithm which was developed is presented in Appendix B. Several features need to be discussed. Starting from the top of the chart, an option is included for making a specifiable number of runs of the program merely by stacking the input data decks. Variables are initialized and a table of linear attenuation coefficient versus photon energy is constructed for both materials. These tables are interpolated for coefficients at the scattered energy later on in the calculation. A timer is set in motion and a run is started. An outer loop increments the independent variable, and an eight-way branch differentiates between the eight cases the program will handle. The eight cases

are: detector response versus α_d , D_d , β_d , A , t , E_ν , or N ; and run time versus an optimizing parameter, N_{rpt} , which is used as a dead-end criterion later on. The next inner loop generates a representative sample of paths using Monte Carlo sampling techniques as outlined in the preceding section. The optimizing parameter, N_{rpt} , is used in this step as follows: The photon path is generated in sequence from the source to the interaction point. If this point is not in the detector cone, new interaction points are generated by regenerating the penetration distance, p , for N_{rpt} trials. If an interaction point is still not found within the detector cone, the routine goes back and regenerates the target surface intercept, thereby changing the incident direction. This device lowers the execution time considerably because the target surface intercept is much more time consuming to generate than the penetration distance. The best value for the optimizing parameter can be found by taking the worst-case geometry for any particular run and making a run for run time versus N_{rpt} . Finally, the loop under discussion calculates the survival probabilities and keeps a running sum as it goes. The timer is checked to see that the specified time is not exceeded, and then the outer loop increments the independent variable. Upon successful completion of a run, the next segment prints out a table of detector response versus the independent variable, and then prepares a graph of the table. This segment allows the option of putting one or several runs on the same graph, and also causes the graph to be made semilog in the X direction when running response versus sample size, N . Plot tapes are generated by a generalized plotting routine called GENPLT,⁽¹²⁾ invoked by a CALL statement in FORTRAN.

A comparison of the computer model with experiment was made for a problem in response versus coating thickness (or DXT, considering the density constant). Figure 3 offers the problem setup, and Figure 4 a graphical comparison. The computer model reproduces all qualitative aspects of the experimental curve. The model curve was normalized to the Y-axis intercept of the experimental curve.

CONCLUSIONS AND RECOMMENDATIONS

Results given here indicate that the Compton scattering process can be represented qualitatively to a useful degree of accuracy by considering only single scattering in the Compton-dominant region. In typical geometries, a Monte Carlo sample of about 100 - 300 paths is adequate to represent the action of the source beam in the material. Running times for the computer program range from two to twenty minutes, with four minutes being typical on an IBM 360-50/65 computer.

Figure 3. AN EXPERIMENTALLY RUN PROBLEM..

Figure 4. DETECTOR RESPONSE AS A FUNCTION OF THE COATING THICKNESS FOR STEEL ON ALUMINUM. (Comparison of the Model with the Experimentally Run Problem)

Compton scattering is only one of several important interactions. Some of the others, among them fluorescence and coherent scattering, show promise of yielding to the same type of analysis as that used in this report. The sample of interaction points generated in this model is based on a total interaction (minus coherent) cross section, so that the calculation could be expanded from the interaction points to follow another process instead of or in addition to Compton scattering.

Some work has been done along this line toward including a fluorescence correction along with Compton scattering. All the logistics for handling a first-order fluorescence correction, including a subroutine which generates detector points with uniform angular distribution about the interaction points, are built into the program. What remains to be done is the development of a suitable expression for the probability that a gamma from the source will trigger a sequence of events resulting in an X-ray intercepting the detector.

REFERENCES

- (1) Kahn, H.; Applications of Monte Carlo, RM-1237-AEC; The RAND Corporation, Palo Alto, California (1956).
- (2) Evans, R. D.; The Atomic Nucleus, p 712; McGraw-Hill Book Company, New York, New York (1955).
- (3) Ibid, pp 672-693.
- (4) Fano, U.; "Gamma-Ray Attenuation, Part I: Basic Processes", Nucleonics, 11, pp 8 - 12; August 1953.
- (5) Fano, U.; "Gamma-Ray Attenuation, Part II: Analysis of Penetration", Nucleonics, 11, pp 55 - 61; September 1953.
- (6) Davisson, C. M. and Evans, R. D.; "Gamma-Ray Absorption Coefficients", Revs Mod Phys, 24, pp 79 - 107; April 1952.
- (7) Pratt, R.; Theory of Gamma-Ray Cross Sections, NYO-3829-17; University of Pittsburgh, Pittsburgh, Pennsylvania; November 1967.
- (8) Storm, E. and Israel, H.; Photon Cross Sections from 0.001 to 100 Mev for Elements 1 Through 100, LA-3753; Los Alamos Scientific Laboratory; June 1967.
- (9) Hubbell, J. H.; Photon Cross Sections, Attenuation Coefficients, and Energy Absorption Coefficients from 10 Kev to 100 Gev, NSRDS-NBS-29; US National Bureau of Standards, Washington, DC; August 1969.
- (10) McMaster, W. H., Del Grande, N. K., Mallett, J. H., and Hubbell, J. H.; Compilation of X-Ray Cross Sections, UCRL-50174, Sections I-IV; Lawrence Radiation Laboratory, Livermore, California; January 1970.
- (11) Hammersley, J. M. and Handscomb, D. C.; Monte Carlo Methods, p 36; Methuen and Company, Limited, London (1964).
- (12) Computing Technology Center IBM 360 Programmer's Notebook, Section XVIII, p 25; Union Carbide Corporation-Nuclear Division, Oak Ridge, Tennessee (1970).

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APPENDIX A

MATHEMATICAL DERIVATIONS

Source Point

Assume that a routine for generating random numbers from a uniform distribution is available, denoted by:

$$0 \leq r_i \leq 1.$$

Consider the following geometry:

then generate:

$$x'_s = R_s (2r_i - 1), \text{ and}$$

$$z'_s = R_s (2r_i - 1).$$

If $(x'_s)^2 + (z'_s)^2 \leq R_s^2$, accept; if not, reject and regenerate x'_s and z'_s .

Translate the accepted point to the source plane:

where:

$$x_s = D_s \cos \alpha_s + x'_s \sin \alpha_s,$$

$$y_s = D_s \sin \alpha_s - x'_s \cos \alpha_s, \text{ and}$$

$$z_s = z'_s.$$

The efficiency of this process is expressed by:

$$e = \frac{\text{area of disc}}{\text{area of enclosing square}} = \frac{\pi R_s^2}{4R_s^2} = \frac{\pi}{4}.$$

Equation of the Source Cone

From:

the equation of a cone can be expressed as:

$$r' = R_s - \frac{R_s}{(H_s - D_s)} (y' - D_s) = R_s - (y' - D_s) \tan \beta_s, \text{ and}$$

$$(x')^2 + (z')^2 = \left[R_s - (y' - D_s) \tan \beta_s \right]^2.$$

If the cone is tilted to the source axis, the transformation is:

$$x' = x \sin \alpha_s - y \cos \alpha_s ,$$

$$y' = x \cos \alpha_s - y \sin \alpha_s , \text{ and}$$

$$z' = z .$$

Hence, the equation of the source cone becomes:

$$(x \sin \alpha_s - y \cos \alpha_s)^2 + z^2 = [R_s - (x \cos \alpha_s + y \sin \alpha_s - D_s) \tan \beta_s]^2 .$$

Equation of the Detector Cone

From:

and analogously to the source cone derivation:

$$(x')^2 + (z')^2 = [R_d - (y' - D_d) \tan \beta_d]^2 .$$

If this expression is translated and rotated to the detector axis, the transformation becomes:

$$x' = (x + A) \sin \alpha_d + y \cos \alpha_d ,$$

$$y' = -(x + A) \cos \alpha_d + y \sin \alpha_d , \text{ and}$$

$$z' = z .$$

Hence, the equation of the detector cone is:

$$\left[(x + A) \sin \alpha_d + y \cos \alpha_d \right]^2 + z^2 = \left\{ R_d - \left[- (x + A) \cos \alpha_d + y \sin \alpha_d - D_d \right] \tan \beta_d \right\}^2.$$

Target Surface Seen by the Source

This area is the intersection of the plane, $y = 0$, and the source cone:

$$(x \sin \alpha_s)^2 + z^2 = \left[R_s - (x \cos \alpha_s - D_s) \tan \beta_s \right]^2.$$

This area is an elliptical conic section.

Target Surface Seen by the Detector

This area is the intersection of the plane, $y = 0$, and the detector cone:

$$\left[(x + A) \sin \alpha_d \right]^2 + z^2 = \left\{ R_d - \left[- (x + A) \cos \alpha_d - D_d \right] \tan \beta_d \right\}^2.$$

This area is an elliptical conic section.

$1/r^2$ Intensity Variation

First, calculate the minimum distance, $r_{\min}$, which can occur:

Thus:

$$r_{\min}^2 = (x_2 - x_1)^2 + y_1^2, \text{ in either case.}$$

Source:

$$x_1 = D_s \cos \alpha_s + R_s \sin \alpha_s,$$

$$y_1 = D_s \sin \alpha_s - R_s \cos \alpha_s, \text{ and}$$

$$0 \leq \alpha_s \leq \frac{\pi}{2}.$$

The value of x_2 for the source is found from the equation for the target surface seen by the source, with $z = 0$:

$$(x_2 \sin \alpha_s)^2 = [R_s - (x_2 \cos \alpha_s - D_s) \tan \beta_s]^2,$$

$$\pm x_2 \sin \alpha_s = R_s - (x_2 \cos \alpha_s - D_s) \tan \beta_s,$$

$$x_2 (\cos \alpha_s \tan \beta_s \pm \sin \alpha_s) = R_s + D_s \tan \beta_s, \text{ and}$$

$$x_2 = \frac{R_s + D_s \tan \beta_s}{\cos \alpha_s \tan \beta_s \pm \sin \alpha_s}.$$

To determine the correct sign, when:

$$\alpha_s = \frac{\pi}{2}, \text{ and}$$

$$\beta_s = 0,$$

must have:

$$x_2 = R_s;$$

hence,

$$x_2 = \frac{R_s + D_s \tan \beta_s}{\cos \alpha_s \tan \beta_s + \sin \alpha_s}.$$

Detector:

$$x_1 = -D_d \cos \alpha_d - R_d \sin \alpha_d,$$

$$y_1 = D_d \sin \alpha_d - R_d \cos \alpha_d, \text{ and}$$

$$0 \leq \alpha_d \leq \frac{\pi}{2}.$$

The value of x_2 for the detector is found analogously to the value for the source, except that the detector value is translated by A:

$$x_2 = -A - \frac{R_d + D_d \tan \beta_d}{\cos \alpha_d \tan \beta_d + \sin \alpha_d}.$$

Now, if a source of uniform random numbers, r_i , is available, the rejection technique is as follows:

1. Calculate $P_1 = 1/r^2$ for the given distance r .
2. Calculate $P_2 = r_i/r_{\min}^2$, $0 \leq r_i \leq 1$.
3. If $P_2 > P_1$, reject r ; otherwise accept.

If some $r_{\max}$ is the maximum expected distance, the efficiency of the process just derived can be found from the following considerations:

$$e = \frac{\text{area under curve}}{\text{area of rectangle}} = \frac{\int_{r_{\min}}^{r_{\max}} \frac{dr}{r}}{\frac{1}{r_{\min}} (r_{\max} - r_{\min})}, \text{ or}$$

$$e = \frac{r_{\min} \ln \left(\frac{r_{\max}}{r_{\min}} \right)}{(r_{\max} - r_{\min})}.$$

Obviously, the expression must have:

$$r_{\max} \neq 0, \text{ and}$$

$$r_{\min} \neq 0.$$

The efficiency goes down as $r_{\min} \rightarrow 0$, because:

$$\lim_{r_{\min} \rightarrow 0} e = \lim_{r_{\min} \rightarrow 0} \left\{ \frac{\ln r_{\max} - \ln r_{\min}}{\left(\frac{r_{\max}}{r_{\min}} - 1 \right)} \right\} = \lim_{r_{\min} \rightarrow 0} \left\{ - \frac{r_{\min}}{r_{\max}} \right\} \equiv 0.$$

Uniform Target Surface Points

From the equation for the target surface seen by the source, the illuminated area is bounded by:

$$(x \sin \alpha_s)^2 + z^2 = \left[R_s - (x \cos \alpha_s - D_s) \tan \beta_s \right]^2.$$

This expression can be rearranged into the form for the standard ellipse:

$$\begin{aligned} (x \sin \alpha_s)^2 + z^2 &= \left[(R_s + D_s \tan \beta_s) - x \tan \beta_s \cos \alpha_s \right]^2, \text{ or} \\ &= (R_s + D_s \tan \beta_s)^2 - 2x (R_s + D_s \tan \beta_s) \tan \beta_s \cos \alpha_s + x^2 (\tan \beta_s \cos \alpha_s)^2. \end{aligned}$$

And:

$$x^2 \left(\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s \right) + x \left[2 (R_s + D_s \tan \beta_s) \tan \beta_s \cos \alpha_s \right] + z^2 = (R_s + D_s \tan \beta_s)^2.$$

Completing the square in x , this expression becomes:

$$\left[x + \frac{(R_s + D_s \tan \beta_s) \cos \alpha_s \tan \beta_s}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s} \right]^2 + \left[\frac{z^2}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s} \right] = \left[\frac{(R_s + D_s \tan \beta_s)^2}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s} \right] + \left[\frac{(R_s + D_s \tan \beta_s) \tan \beta_s \cos \alpha_s}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s} \right]^2.$$

If the standard form is:

$$\frac{(x - h)^2}{a^2} + \frac{z^2}{b^2} = 1,$$

then:

$$h = - \frac{(R_s + D_s \tan \beta_s) \tan \beta_s \cos \alpha_s}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s},$$

$$a^2 = \frac{(R_s + D_s \tan \beta_s)^2}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s} \left[1 + \frac{\tan^2 \beta_s \cos^2 \alpha_s}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s} \right], \text{ and}$$

$$b^2 = (R_s + D_s \tan \beta_s)^2 \left[1 + \frac{\tan^2 \beta_s \cos^2 \alpha_s}{\sin^2 \alpha_s - \tan^2 \beta_s \cos^2 \alpha_s} \right].$$

Uniform random points on the rectangle enclosing this ellipse are generated as follows:

$$x_T = a (2r_i - 1) + h,$$

$$z_T = b (2r_i - 1).$$

If the point is also inside the ellipse:

$$\frac{(x_T - h)^2}{a^2} + \frac{z_T^2}{b^2} \leq 1,$$

accept; otherwise, reject and regenerate x_T, z_T .

The points so generated may be weighted with a $1/r^2$ intensity variation about any source point by calculating the distance from the source point to the target point and applying the $1/r^2$ distribution via the rejection technique discussed previously.

Angle of Intercept of the Source Vector with the Target Surface

From:

$$\vec{r}_1 = \hat{i} (x_T - x_s) + \hat{j} (0 - y_s) + \hat{k} (z_T - z_s), \text{ and}$$

$$\vec{r}_2 = \hat{i} (x_T - x_s) + \hat{k} (z_T - z_s).$$

Then:

$$\cos \xi = \frac{\vec{r}_1 \cdot \vec{r}_2}{|\vec{r}_1| |\vec{r}_2|} =$$

$$\frac{(x_T - x_s)^2 + (z_T - z_s)^2}{\left\{ [(x_T - x_s)^2 + y_s^2 + (z_T - z_s)^2] [(x_T - x_s)^2 + (z_T - z_s)^2] \right\}^{1/2}}, \text{ and}$$

$$\cos \xi = \left[\frac{(x_T - x_s)^2 + (z_T - z_s)^2}{(x_T - x_s)^2 + y_s^2 + (z_T - z_s)^2} \right], \quad 0 \leq \xi \leq \frac{\pi}{2}.$$

Penetration Distance

This distance can be calculated at random directly from the known intensity variation with depth:

The probability density function would then be:

$$f(x) = \begin{cases} A_1 e^{-\mu_{11}x} & 0 \leq x \leq t/\sin\xi \\ A_1 e^{-(\mu_{11} - \mu_{21})t/\sin\xi} e^{-\mu_{21}x} & t/\sin\xi \leq x < \infty \end{cases}$$

Normalization requires that:

$$\int_0^{\infty} f(x) dx = 1, \text{ or}$$

$$A_1 = \frac{1}{\frac{1}{\mu_{11}} + \left(\frac{1}{\mu_{21}} - \frac{1}{\mu_{11}} \right) e^{-\mu_{11}t/\sin\xi}}.$$

The probability distribution is found by integrating $f(x)$:

$$F(x) = \int_0^x A_1 e^{-\mu_{11}x} dx = \frac{A_1}{\mu_{11}} \left[1 - e^{-\mu_{11}x} \right], \text{ or}$$

$$0 \leq x \leq t/\sin\xi$$

$$F(x) = \int_0^{t/\sin\xi} A_1 e^{-\mu_{11}x} dx + \int_{t/\sin\xi}^x A_1 e^{-(\mu_{11} - \mu_{21})t/\sin\xi} e^{-\mu_{21}x} dx, \text{ or}$$

$$F(x) = \frac{A_1}{\mu_{11}} \left[1 - e^{-\mu_{11}t/\sin\xi} \right] +$$

$$\frac{A_1}{\mu_{21}} e^{-(\mu_{11} - \mu_{21})t/\sin\xi} \left[e^{-\mu_{21}t/\sin\xi} - e^{-\mu_{21}x} \right].$$

$$t/\sin\xi \leq x < \infty$$

Random values of x with this distribution can be found by setting:

$$F(x) = r_i,$$

where r_i is a random number from a uniform distribution.

Solving the last equation for x in terms of r_i gives:

$$x_i = -\frac{1}{\mu_{11}} \ln \left(1 - \frac{\mu_{11} r_i}{A_1} \right) \text{ if } 0 \leq r_i \leq \frac{A_1}{\mu_{11}} \left(1 - e^{-\mu_{11} t / \sin \xi} \right), \text{ or}$$

$$x_i = -\frac{1}{\mu_{21}} \ln \left\{ \frac{\mu_{21}}{A_1} e^{(\mu_{11} - \mu_{21}) t / \sin \xi} [1 - r_i] \right\}$$

$$\text{if } \frac{A_1}{\mu_{11}} \left(1 - e^{-\mu_{11} t / \sin \xi} \right) \leq r_i \leq 1 - \frac{A_1}{\mu_{21}} e^{-[\mu_{21} d_{\max} + (\mu_{11} - \mu_{21}) t] / \sin \xi}.$$

The factor, $\mu_{21} d_{\max}$, appears in the exponent in the last inequality so as to limit the penetration distance to $\leq d_{\max} / \sin \xi$ (no penetration completely through the substrate). If r_i' is a source of uniform random numbers ($0 \leq r_i' \leq 1$), then r_i is generated from:

$$r_i = r_i' \left\{ 1 - \frac{A_1}{\mu_{21}} e^{-[\mu_{21} d_{\max} + (\mu_{11} - \mu_{21}) t] / \sin \xi} \right\}.$$

Coordinates of the Interaction Point

From:

It is seen by inspection:

$$y_p = -p \sin \xi, \text{ and}$$

$$x_p = x_T + p \cos \xi \frac{\hat{i}(x_T - x_s) + \hat{k}(z_T - z_s)] \cdot \hat{i}}{\left[(x_T - x_s)^2 + (z_T - z_s)^2\right]^{1/2}}, \text{ or}$$

$$x_p = x_T + \frac{p(x_T - x_s) \cos \xi}{\left[(x_T - x_s)^2 + (z_T - z_s)^2\right]^{1/2}}.$$

Analogously:

$$z_p = z_T + \frac{p(z_T - z_s) \cos \xi}{\left[(x_T - x_s)^2 + (z_T - z_s)^2\right]^{1/2}}.$$

Acceptance of the Interaction Point

Only a point within both the source and detector cones can be accepted. From the equations for the two cones, the criteria for acceptance are:

$$(x_p \sin \alpha_s - y_p \cos \alpha_s)^2 + z_p^2 \leq [R_s - (x_p \cos \alpha_s + y_p \sin \alpha_s - D_s) \tan \beta_s]^2, \text{ and}$$

$$\begin{aligned} & [(x_p + A) \sin \alpha_d + y_p \cos \alpha_d]^2 + \\ & z_p^2 \leq \left\{ R_d - [-(x_p + A) \cos \alpha_d + y_p \sin \alpha_d - D_d] \tan \beta_d \right\}^2. \end{aligned}$$

Uniform Detector Points

The coordinates are derived the same as for the source:

$$x_d' = R_d (2r_i - 1), \text{ and}$$

$$z_d' = R_d (2r_i - 1).$$

$$(x_d')^2 + (z_d')^2 \leq R_d^2, \text{ accept.}$$

Then:

$$x_d = -D_d \cos \alpha_d + x_d' \sin \alpha_d,$$

$$y_d = D_d \sin \alpha_d + x_d' \cos \alpha_d, \text{ and}$$

$$z_d = z_d'.$$

Distances d_t and d_{esc} Along the Exit Path

From:

The equation of the line joining the interaction and detector points is:

$$(x - x_p) \left(\frac{z_d - z_p}{x_d - x_p} \right) = (y - y_p) \left(\frac{z_d - z_p}{y_d - y_p} \right) = (z - z_p).$$

The intersection of this line and the plane, $y = 0$, is at:

$$(x - x_p) \frac{(z_d - z_p)}{(x_d - x_p)} = -y_p \frac{(z_d - z_p)}{(y_d - y_p)}, \text{ and}$$

$$x_{TE} = x_p - y_p \left(\frac{x_d - x_p}{y_d - y_p} \right).$$

Further:

$$-y_p \left(\frac{z_d - z_p}{y_d - y_p} \right) = (z - z_p), \text{ and}$$

$$z_{TE} = z_p - y_p \left(\frac{z_d - z_p}{y_d - y_p} \right).$$

The intersection of the line and the plane, $y = -t$, is at:

$$(x - x_p) \frac{(z_d - z_p)}{(x_d - x_p)} = (-t - y_p) \frac{(z_d - z_p)}{(y_d - y_p)},$$

$$x_{TT} = x_p - (t + y_p) \left(\frac{x_d - x_p}{y_d - y_p} \right),$$

$$(-t - y_p) \left(\frac{z_d - z_p}{y_d - y_p} \right) = (z - z_p), \text{ and}$$

$$z_{TT} = z_p - (t + y_p) \left(\frac{z_d - z_p}{y_d - y_p} \right).$$

The distances then follow directly:

$$d_t^2 = (x_{TT} - x_p)^2 + (-t - y_p)^2 + (z_{TT} - z_p)^2, \text{ and}$$

$$d_{esc}^2 = (x_{TE} - x_p)^2 + y_p^2 + (z_{TE} - z_p)^2.$$

Compton Angle

From:

$$\vec{r}_1 = \hat{i}(x_p - x_s) + \hat{j}(y_p - y_s) + \hat{k}(z_p - z_s), \text{ and}$$

$$\vec{r}_2 = \hat{i}(x_d - x_p) + \hat{j}(y_d - y_p) + \hat{k}(z_d - z_p).$$

Also:

$$\cos \theta = \frac{\vec{r}_1 \cdot \vec{r}_2}{|\vec{r}_1| |\vec{r}_2|}.$$

Thus:

$$\cos \theta = \frac{(x_p - x_s)(x_d - x_p) + (y_p - y_s)(y_d - y_p) + (z_p - z_s)(z_d - z_p)}{\left\{ \left[(x_p - x_s)^2 + (y_p - y_s)^2 + (z_p - z_s)^2 \right] \left[(x_d - x_p)^2 + (y_d - y_p)^2 + (z_d - z_p)^2 \right] \right\}^{1/2}}.$$

Having the Compton angle, use the Klein-Nishima formula to force a proper distribution of detector points by rejection.

If:

$$\mu = \cos \theta, \text{ and}$$

$$\alpha = h\nu/mc^2,$$

then:

$$p(\mu) = \frac{d\sigma}{\sigma} = \frac{d\Omega}{4\pi} \frac{\left\{ \frac{1+\mu^2}{[1+\alpha(1-\mu)]^2} + \frac{\alpha^2(1-\mu)^2}{[1+\alpha(1-\mu)]^3} \right\}}{\left\{ \left(\frac{1+\alpha}{\alpha^2} \right) \left[\frac{2(1+\alpha)}{1+2\alpha} - \frac{1}{\alpha} \ln(1+2\alpha) \right] + \frac{\ln(1+2\alpha)}{2\alpha} - \frac{1+3\alpha}{(1+2\alpha)^2} \right\}}.$$

Calculate:

$$p_i = p(1) r_i$$

$0 \leq r_i \leq 1$ (uniform), and

$$p_i = p(\cos \theta_i).$$

If:

$$p_i \leq p_i, \text{ accept } \cos \theta_i;$$

otherwise reject and regenerate $\cos \theta$.

APPENDIX B

FLOW CHART FOR THE COMPUTER PROGRAM

APPENDIX C

FORTRAN LISTING OF THE COMPUTER PROGRAM

Control Cards (IBM 360-50/65)

```
//YY#CMD30 JOB                DAVENPORT,MSGLEVEL=1,CLASS=C,REGION=200K
/*SETUP DDNAME=FT15F001,DEVICE=TAPE7,ID=(SCRATCH,RING,SAVE,SL)
//STD EXEC PGM=PLTSTART
//FT15F001 DD LABEL=(1,SL),UNIT=TAPE7
//STEP1 EXEC FORTHCLG,PARM,FORT='NOMAP',PARM.LKED=(),GOTIME=8
//FORT.SYSIN DD *
/*
//GO.FT15F001 DD LABEL=(1,SL),UNIT=TAPE7
//GO.FT05F001 DD *
/*
/*
```

Main Program

```
REAL DFLAG*8(6)/0.D0,1.D0,2*0.D0,1.D0,0.D0/
REAL TOP(21)/72.,.1,.175,18*4H /
REAL BOTTOM(21)/72.,.1,.175,18*4H /
REAL SIDE(13)/40.,.1,.175,'RELA','TIVE','RES','PONS','E OF',
1 'A L','INEA','R DE','TECT','OR ' /
DIMENSION XPM(50),YRESP(50)
DIMENSION TBL1(501),TBL2(501)
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,NMAX,SN7,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
READ(5,2)JRUNS,IGR
2 FORMAT(2I10)
DO 110 KJ=1,JRUNS
CALL INPUT
CALL XPRMS(EGAM)
SNAD=SIN(ALPHAD*3.141593/180.)
CNAD=COS(ALPHAD*3.141593/180.)
TNBD=TAN(BETAD*3.141593/180.)
SNAS=SIN(ALPHAS*3.141593/180.)
CNAS=COS(ALPHAS*3.141593/180.)
TNBS=TAN(BETAS*3.141593/180.)
CNAS1=ABS(CNAS)
C1=(RS+DS*TNBS)/(SNAS+CNAS1*TNBS)-(DS*CNAS1+RS*SNAS)
C2=DS*SNAS-RS*CNAS1
RWFTS=1.0/(C1*C1+C2*C2)
CS1=1.
CALL PKN
P1=PRKN
T=0.00254*T
```

```

      DMAX1=DMAX
      DMAX=DMAX+T
      XS=1.
      YS=1.
      ZS=1.
      CALL TSPT
      RA1=0.602257*RHO1/A1
      RA2=0.602257*RHO2/A2
      ALPH=EGAM/0.511
      NE=501
      FNE1=FLOAT(NE-1)
      E11=E1(1)
      E18=E1(8)
      E21=E2(1)
      E28=E2(8)
      DE1=(E18-E11)/FNE1
      DE2=(E28-E21)/FNE1
      CF2=FNE1/E28
      CF1=FNE1/E18
      DO 5 I=1,NE
      FI=I-1
      EI1=E11+FI*DE1
      EI2=E21+FI*DE2
      TBL1(I)=RA1*XSECT(EI1,E1,TL1)
      TBL2(I)=RA2*XSECT(EI2,E2,TL2)
5     CONTINUE
      IF(IPR.EQ.8)GO TO 6
      CALL ITIME(ICLOCK,IDIFF)
      TIME=0.
6     DELP=(PRM2-PRM1)/FLOAT(NPT)
      IPT=NPT+2
      DO 100 I=1,IPT
      PRM=PRM1+FLOAT(I-2)*DELP
      IF(I.GT.1)GO TO 3
      PRM=NORM
      NTRIES=0
3     GO TO(11,13,15,17,19,21,23,18),IPR
11    ALPHAD=PRM*3.141593/180.
      SNAD=SIN(ALPHAD)
      CNAD=COS(ALPHAD)
      GO TO 25
13    DD=PRM
      GO TO 25
15    BETAD=PRM*3.141593/180.
      TNBD=TAN(BETAD)
      GO TO 25
17    A=PRM
      GO TO 25
18    CALL ITIME(ICLOCK,IDIFF)
      NRPT=PRM
      GO TO 25
19    T=PRM*0.00254
      DMAX=DMAX1+T
      GO TO 25
21    EGAM=PRM
      CALL XPRMS(EGAM)
      CALL PKN
      ALPH=EGAM/0.511
      GO TO 25

```

```

23 IF(I.EQ.1)GO TO 22
   READ(5,24)N
24 FORMAT(I4)
   GO TO 26
22 N=NORM
26 PRM=N
25 CONTINUE
   IF(IPR.GT.3)GO TO 27
   CNAD1=ABS(CNAD)
   C1=(RD+DD*TNBD)/((SNAD+CNAD1*TNBD)-(DD*CNAD1+RD*SNAD)
   C2=DD*SNAD-RD*CNAD1
   RWFTD=1.0/(C1*C1+C2*C2)
   PRW=P1*RWFTD
27 SUM=0.
   JSUM=0
   DO 90 J=1,N
28 CALL SPT
31 CALL TSPT1
   ITP=0
32 CNZ=CZETA(1.)
   SNZ=SQRT(1.-CNZ*CNZ)
33 P=PEN(1.)
   ITP=ITP+1
   CALL INTPT
   IF(IPR.EQ.7)GO TO 35
   IF(I.EQ.1)GO TO 34
   IF(JSUM.GT.NTRIES)GO TO 95
   JSUM=JSUM+1
   GO TO 35
34 NTRIES=NTRIES+1
35 XA=XP-A
   AA1=XA*SNAD+YP*CNAD
   B=RD+(XA*CNAD-YP*SNAD+DD)*TNBD
   DCONE=(AA1*AA1+ZP*ZP)/(B*B)
   IF(DCONE.GT.1.)GO TO 40
   GO TO 36
40 IF(ITP.GT.NRPT)GO TO 31
   GO TO 33
36 CALL DPTC
   IF(RUNTP.EQ.2)CALL DPTF
88 EESC=EGAM/(1.+ALPH*(1.-CS1))
   IE1=EESC*CF1+1.5
   IE2=EESC*CF2+1.5
   M12=TBL1(IE1)
   M22=TBL2(IE2)
   CALL EXITD
   PROB=PPTH(XX)
90 SUM=SUM+PROB
95 XPM(I)=PRM
   YRESP(I)=SUM
   IF(IPR.EQ.8)GO TO 98
   IF(IPR.EQ.7)YRESP(I)=SUM/FLOAT(N)
   GO TO 99
96 FORMAT(1X,1P2E12.3)
98 CALL ITIME(ICLOCK,IDIFF)
   YRESP(I)=FLOAT(IDIFF)/FLOAT(100*N)
   GO TO 100
99 CALL ITIME(ICLOCK,IDIFF)
   TIME=TIME+FLOAT(IDIFF)

```

```

      IF (TIME.LT.T1) GO TO 100
      IPT=I
      WRITE(6,107)
107  FORMAT(1X,'RUN ENDING BECAUSE SPECIFIED EXECUTION TIME WAS EXCEED
      1D')
      GO TO 101
100  CONTINUE
101  YNORM=YRESP(1)
      IF (IPR.EQ.8) GO TO 103
      DO 102 I=1,IPT
102  YRESP(I)=YRESP(I)/YNORM
      GO TO 104
103  READ(5,106)(SIDE(I),I=4,13)
104  READ(5,105)(TOP(I),I=4,21)
      READ(5,105)(BOTTOM(I),I=4,21)
105  FORMAT(18A4)
106  FORMAT(10A4)
      WRITE(6,130)IPR
130  FORMAT(2X,'PARAMETER ',I1,4X,'RESPONSE')
      WRITE(6,96)(XPM(I),YRESP(I),I=1,IPT)
      ITYPE=4
      IF (IPR.EQ.7) ITYPE=1
      IF (IGR.EQ.2) GO TO 125
      CALL GENPLT(IPT,XPM,YRESP,10.,8.,DFLAG,TOP,BOTTOM,SIDE,ITYPE)
      CALL NEWPIC
      GO TO 110
125  IF (KJ.EQ.1) GO TO 108
      CALL GENPT(XPM,YRESP,IPT,0)
      GO TO 110
108  CALL GENPLT(IPT,XPM,YRESP,10.,8.,DFLAG,TOP,BOTTOM,ITYPE)
110  IF (IGR.EQ.2) CALL NEWPIC
      CALL STOP
      STOP
      FND

```

Subroutines

```

SUBROUTINE INPUT
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1  EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2  IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3  TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4  CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5  PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6  M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
DIMENSION TITLE(18)
READ(5,40)(TITLE(I),I=1,18)
40  FORMAT(18A4)
READ(5,19)RUNTYP,FYLD,SKEDG
19  FORMAT(I10,2F10.0)
READ(5,16)IPR,PRM1,PRM2,NORM,NPT,N
16  FORMAT(I10,3F10.0,2I10)
READ(5,35)UNIT,UNIT1,UNID,UNID1,NRPT,T1
35  FORMAT(A4,I6,A4,I6,I10,F10.0)
WRITE(6,15)(TITLE(I),I=1,18),IPR,NRPT,T1,PRM1,PRM2,NORM,NPT,UNIT,
1  N,UNID

```

```

15 FORMAT(1X,'INPUT LISTING',5X,18A4,/,1X,'CODE FOR PARAMETER TO BE
1VARIED:',14,15X,'OPTIMIZING PARAMETER:',14,5X,'TIME LIMIT, MINUTES
1:', F5.1,/,1X,'RANGE:',F8.2,' TO',F8.2,25X,'NORMALIZE TO RESPON
1E AT:',F8.2,/,1X,'NO. OF POINTS TO BE CALCULATED:',14,16X,'ASSUME
1 UNIFORM TARGET ILLUMINATION?',1X,A4,/,1X,' NO. OF EVENTS AT NORMAL I
1ZING POINT:',16,10X,'ASSUME UNIFORM DETECTOR ILLUMINATION?',1X,A4)
T1=T1*6000.
READ(5,17)RS,BETAS,DS,ALPHAS
17 FORMAT(4F10.0)
READ(5,18)RD,BETAD,DD,ALPHAD,A,DMAX,T
18 FORMAT(7F10.0)
WRITE(6,2)
2 FORMAT(1X,/,1X,'GEOMETRY PARAMETERS',/)
WRITE(6,3)RS,BETAS,DS,ALPHAS,RD,BETAD,DD,ALPHAD,A,DMAX,T
3 FORMAT(1X,' RS',3X,F10.2,/,1X,'BETA S',3X,F10.2,/,1X,
1 ' DS',3X,F10.2,/,1X,'ALPHAS',3X,F10.2,/,1X,' RD',
2 3X,F10.2,/,1X,'BETA D',3X,F10.2,/,1X,' DD',3X,
3 F10.2,/,1X,'ALPHAD',3X,F10.2,/,1X,' A',3X,F10.2,/,
4 1X,' D MAX',3X,F10.2,/,1X,' T',3X,F10.2,/)
READ(5,17)A1,RHO1,A2,RHO2
WRITE(6,4)
4 FORMAT(1X,'MATERIAL PROPERTIES',/)
WRITE(6,5)A1,RHO1,A2,RHO2
5 FORMAT(1X,' A1',3X,F10.3,/,1X,' RHO1',3X,F10.1,
1 /,1X,' A2',3X,F10.3,/,1X,' RHO2',3X,F10.1,/)
6 READ(5,17)(E1(L),S1(L),TLA(L),TL1(L),L=1,10)
8 WRITE(6,9)
9 FORMAT(1X,'MEDIUM 1 CROSS SECTION VALUES',/,
1 8X,'E',6X,'C SCAT',4X,'ABSORP',5X,'TOTAL')
WRITE(6,10)(E1(I),S1(I),TLA(I),TL1(I),I=1,10)
10 FORMAT(1X,4F10.3)
READ(5,20)(E2(L),S2(L),TL2(L),L=1,10)
20 FORMAT(3F10.0)
12 READ(5,21)EBRK,EGAM
21 FORMAT(2F10.0)
WRITE(6,13)
13 FORMAT(' MEDIUM 2')
WRITE(6,22)(E2(I),S2(I),TL2(I),I=1,10)
22 FORMAT(1X,3F10.3)
WRITE(6,14)EBRK,EGAM
14 FORMAT(1X,/,1X,'EBRK = ',F6.3,/,1X,'EGAM = ',F6.3)
RETURN
END

```

```

FUNCTION RNDM(X)
DATA IX/13254769/
IY=IX*65539
IF(IY)5,6,6
5 IY=IY+2147483647+1
6 RNDM=IY
RNDM=RNDM*0.4656613E-9
IX=IY
RETURN
END

```

```

SUBROUTINE SPT
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
10 X=RS*(2.0*RNDM(1.))-1.)
Z=RS*(2.0*RNDM(2.))-1.)
IF((X*X+Z*Z).GT.(RS*RS))GO TO 10
XS=DS*CNAS+X*SNAS
YS=DS*SNAS-X*CNAS
ZS=Z
RETURN
END

```

```

SUBROUTINE XPRMS(E)
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
REAL N1
INTEGER UNIT1,UNID1,RUNTYP
N1=.602257
SC11=XSECT(E,E1,S1)
TL11=XSECT(E,E1,TL1)
M11=RHO1*N1*TL11/A1
SC21=XSECT(E,E2,S2)
TL21=XSECT(E,E2,TL2)
M21=RHO2*N1*TL21/A2
M12F=RHO1*N1*SKEDG/A1
RETURN
END

```

```

SUBROUTINE TSPT
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
A3=CNAS*TNBS
A4=RS+DS*TNBS
A5=A4*A4
A6=SNAS*SNAS-A3*A3
A7=A5/A6
A8=A3

```

```

ASQ=A7*(1.+A8*A8/A6)
SASQ=SQRT(ASQ)
BSQ=A5+A7*A8*A8
SBSQ=SQRT(BSQ)
H=-A8*A4/A6
ENTRY TSPT1
XT=SASQ*(2.0*RNDM(1.))-1.)
ZT=SBSQ*(2.0*RNDM(1.))-1.)
IF((XT*XT/ASQ+ZT*ZT/BSQ).GT.1.)GO TO 5
XT=XT+H
IF(UNIT1.EQ.1)RETURN
X=XT-XS
Z=ZT-ZS
PI=RWFTS*RNDM(3.)
PJ=1.0/(X*X+Y*Y+Z*Z)
IF(PI.GT.PJ)GO TO 5
RETURN
END

```

```

FUNCTION CZETA(XX)
COMMON/VBLS/R,S,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
XTS=XT-XS
ZTS=ZT-ZS
XTS=XTS*XTS
ZTS=ZTS*ZTS
CZETA=SQRT((XTS+ZTS)/(XTS+YS*YS+ZTS))
RETURN
END

```

```

FUNCTION PEN(XX)
COMMON/VBLS/R,S,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
AA=1./M11
AB=1./M21
A3=M11*T/SNZ
A4=EXP(-A3)
A5=M21*T/SNZ
A6=EXP(-A5)
A10=1./(AA+(AB-AA)*A4)
A11=A10*AA*(1.-A4)
A12=1.-A10*AB*EXP(-M21*DMAX/SNZ-A3+A5)
5 RI=RNDM(1.)*A12
IF(RI.GT.A11)GO TO 10

```



```

PEN=-AA*ALOG(1.-M11*RI/A10)
RETURN
10 PEN=-AB*ALOG(M21*A6*(1.-RI)/(A10*A4))
RETURN
END

```

```

SUBROUTINE INTPT
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
XTS=XT-XS
ZTS=ZT-ZS
SQXZ=1./SQRT(XTS*XTS+ZTS*ZTS)
UXZ=P*CNZ*SQXZ
XP=XT+XTS*UXZ
YP=-P*SNZ
ZP=ZT+ZTS*UXZ
RETURN
END

```

```

SUBROUTINE DPTF
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
10 X=RD*(2.0*RNDM(1.))-1.)
Z=RD*(2.0*RNDM(2.))-1.)
IF((X*X+Z*Z).GT.(RD*RD))GO TO 10
XDF=-DD*CNAD+X*SNAD
YDF=DD*SNAD+X*CNAD
ZDF=Z
IF(UNID1.EQ.1)RETURN
X=XDF-XP
Y=YDF-YP
Z=ZDF-ZP
PI=RWFTD*RNDM(3.)
PJ=1.0/(X*X+Y*Y+Z*Z)
IF(PI.GT.PJ)GO TO 10
RETURN
END

```

```

SUBROUTINE DPTC
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,

```

```

5  PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6  M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
10 X=RD*(2.0*RNDM(1.)-1.)
Z=RD*(2.0*RNDM(2.)-1.)
IF((X*X+Z*Z).GT.(RD*RD))GO TO 10

XD=-DD*CNAD+X*SNAD
YD=DD*SNAD+X*CNAD
ZD=Z
CS1=CSTH(1.)
IF(UNID1.EQ.1)RETURN
X=XD-XP
Y=YD-YP
Z=ZD-ZP
CALL PKN1
PI=PRW*RNDM(1.)
PJ=PRKN/(X*X+Y*Y+Z*Z)
IF(PI.GT.PJ)GO TO 10
RETURN
END

```

```

SUBROUTINE EXITD
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1  EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2  IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3  TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4  CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5  PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6  M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
IF(P*SNZ.GT.T.OR.RUNTYP.EQ.1)GO TO 2
XDFF=XDF-XP
YDFP=YDF-YP
ZDFP=ZDF-ZP
X=-YP*XDFF/YDFP
Z=-YP*ZDFP/YDFP
DESCF=SQRT(X*X+YP*YP+Z*Z)
2 XDP=XD-XP
YDP=YD-YP
ZDP=ZD-ZP
X=-YP*XDP/YDP
Z=-YP*ZDP/YDP
DESC=SQRT(X*X+YP*YP+Z*Z)
IF(T.EQ.0.)GO TO 5
TYP=T+YP
X=-TYP*XDP/YDP
Z=-TYP*ZDP/YDP
DT=SQRT(X*X+TYP*TYP+Z*Z)
RETURN
5 DT=DESC
DESCF=0.
RETURN
END

```

```

SUBROUTINE PKN
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
ALPHA=EGAM/0.511
AA=1.+ALPHA
AB=AA+ALPHA
A3=AB+ALPHA
A4=1./ALPHA
A5=1./AB
A6=ALOG(AB)
SIGMA=AA*A4*A4*(2.0*AA*A5-A4*A6)+.5*A4*A6-A3*A5*A5
ENTRY PKN1
X2=ALPHA*(1.-CS1)
X3=1.+X2
X4=X2*X3
PRKN=((1.+CS1*CS1)/X4+X2*X2/(X3*X4))/SIGMA
RETURN
END

```

```

FUNCTION Csth(xx)
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
XPS=XP-XS
XDP=XD-XP
YPS=YP-YS
YDP=YD-YP
ZPS=ZP-ZS
ZDP=ZD-ZP
Csth=((XPS*XDP+YPS*YDP+ZPS*ZDP)/SQRT((XPS*XPS+YPS*YPS+ZPS*ZPS)*
1 (XDP*XDP+YDP*YDP+ZDP*ZDP)))
RETURN
END

```

```

FUNCTION PPTH(xx)
COMMON/VBLS/RS,DS,ALPHAS,BETAS,RD,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
CALL PKN1

```

```

IF(P*SNZ.GT.T)GO TO 5
PPTH=(SC11/TL11)*PRKN*EXP(-M11*P-M12*DESC)
IF(RUNTYP.EQ.1)RETURN
PPTH=PPTH+FYLD*((TL11-SC11)/TL11)*EXP(-M11*P-M12F*DESCF)
RETURN
5 PPTH=EXP((M21-M11)*T/SNZ-M21*P-M22*DT-M12*(DESC-DT))
1 *(SC21/TL21)*PRKN
RETURN
END

```

```

FUNCTION XSECT(E,XE,YSCAT)
COMMON/VBLS/RS,DS,ALPHAS,BETAS,3D,DD,ALPHAD,BETAD,A1,RHO1,A2,RHO2,
1 EGAM,E1(10),S1(10),TL1(10),E2(10),S2(10),TL2(10),EBRK,PRM1,PRM2,
2 IPR,XS,YS,ZS,XT,YT,ZT,XP,YP,ZP,XD,YD,ZD,SC11,TL11,M11,SC21,A,
3 TL21,M21,N,DMAX,SNZ,SNAS,CNAS,TNBS,SNAD,CNAD,TNBD,DT,DESC,T,P,
4 CNZ,M12,M22,NORM,JRUNS,UNIT,UNID,NRPT,T1,UNIT1,UNID1,RWFTS,CS1,
5 PRW,RUNTYP,FYLD,SKEDG,XDF,YDF,ZDF,DESCF,M12F,PRKN,RWFTD,NPT,
6 M11F,TLA(10)
REAL M11,M12,M21,M22,NORM,M12F,M11F
INTEGER UNIT1,UNID1,RUNTYP
DIMENSION XE(10),YSCAT(10),C(5),EX(5)
IF(E.GT.EBRK)GO TO 20
DO 5 I=1,5
DENOM=1.
DO 4 J=1,5
IF(J.EQ.I)GO TO 4
DENOM=DENOM*(XE(I)-XE(J))
4 CONTINUE
C(I)=YSCAT(I)/DENOM
5 EX(I)=E-XE(I)
XSECT=0.
DO 8 I=1,5
PROD=1.
DO 6 J=1,5
IF(J.EQ.I)GO TO 6
PROD=PROD*EX(J)
6 CONTINUE
8 XSECT=XSECT+C(I)*PROD
RETURN
20 DO 12 I=1,5
DENOM=1.
DO 10 J=1,5
IF(J.EQ.I)GO TO 10
DENOM=DENOM*(XE(I+5)-XE(J+5))
10 CONTINUE
C(I)=YSCAT(I+5)/DENOM
12 EX(I)=E-XE(I+5)
XSECT=0.
DO 16 I=1,5
PROD=1.
DO 14 J=1,5
IF(J.EQ.I)GO TO 14
PROD=PROD*EX(J)
14 CONTINUE
16 XSECT=XSECT+C(I)*PROD
RETURN
END

```

APPENDIX D

INPUT INSTRUCTIONS

Description of Input Variables

(The input variables are given in the order required on the data input cards.)

<u>Variable Name</u>	<u>Description</u>
JRUNS	Number of separate problem runs in present computer program run.
IGR	The first IGR problem runs will be placed on a single graph.
TITLE(18)	Header line for printout of results.
RUNTYP	Selects types of allowed physical interactions: (1) Compton scatter only, (2) Compton scatter and fluorescence.
FYLD	K-shell fluorescence yield (fraction of events which yield an X ray <u>after a K electron has absorbed a gamma quantum</u>) for the coating.
SKEDG	Total cross section, without coherent scattering, in barns/atom for the coating at an energy just below the K edge.
IPR	Code for the parameter to be varied for the present run:

<u>Code</u>	<u>Parameter</u>
1	α_d
2	D_d
3	β_d
4	A
5	t
6	E_ν
7	N
8	N_{rpt}

PRM1, PRM2	Lower and upper bounds, respectively, of the range over which the parameter designated by IPR is to be varied.
NORM	Value of the independent variable at which the response curve is to be normalized.
NPT	Number of response points to be calculated in the range PRM1, PRM2.
N	Number of paths (Monte Carlo sample size) to be considered at each point on the response curve.
UNIT, UNIT1	<p>Code for target illumination options. If target surface is assumed to be uniformly illuminated by the source, then:</p> <p style="padding-left: 40px;">UNIT = Yes (alphanumeric) UNIT1 = 1</p> <p>Otherwise:</p> <p style="padding-left: 40px;">UNIT = No UNIT1 = 0</p> <p>Where admissible, the YES option allows faster completion of a run.</p>
UNID, UNID1	Code for detector illumination options. (Codes same as for UNIT, UNIT1.)
NRPT	Optimizing parameter specifying the number of times a penetration distance is to be recalculated before the target surface point is recalculated.
T1	Maximum execution time for this problem run. At time T1 the partial results are printed out.
RS	Radius of the disc source, in centimeters.
BETAS	Half angle of the source cone, in degrees.
DS	Distance between source and target surfaces taken along the source cone axis, in centimeters.

ALPHAS	Angle between the target surface and the source cone axis, in degrees.
RD	Radius of the disc detector, in centimeters.
BETAD	Half angle of the detector cone, in degrees.
DD	Distance between detector and target surfaces taken along the detector cone axis, in centimeters.
ALPHAD	Angle between the target surface and the detector cone axis, in degrees.
A	Lateral displacement between the points where the source and detector cone axes intercept the target surface, in centimeters.
DMAX	Thickness of the substrate, in centimeters.
T	Thickness of the coating, in mils.
A1	Atomic weight of the coating, in grams/mole.
RH01	Density of the coating, in grams/cubic centimeter.
A2	Atomic weight of the substrate, in grams/mole.
RH02	Density of the substrate, in grams/cubic centimeter.
E1(i)	Energy entries in the experimental cross section tables for the coating, in million electron volts.
S1(i)	Compton scattering entries in the experimental cross section tables for the coating, in barns/atom.
TLA(i)	Absorption entries in the experimental cross section tables for the coating, in barns/atom.
TL1(i)	Total cross section (minus coherent scattering) entries in the experimental cross section tables for the coating, in barns/atom.
E2(i), S2(i), TL2(i)	Same as for substrate.

EBRK	Energy in million electron volts at the point on the total cross section versus energy curve for the coating which shows the minimum radius of curvature. This value can be a rough estimate. It is used to break the range E1(1), E1(10) into two ranges so that accurate fifth-order Lagrange interpolation for the simulated points is possible.
EGAM	Energy of the source gammas, in million electron volts.
SIDE(13)	Label for the Y axis of the response graph.
TOP(21)	Label for the top of the response graph.
BOTTOM(21)	Label for the X axis of the response graph.

Data Card Formats

The program requires that all variables be identified. Those values not used in a particular run may be given some arbitrary positive value.

Card Number	Input Variables	Format
1	JRUNS, IGR	2I10
2	TITLE(I), I = 1, 18	18A4
3	RUNTYP, FYLD, SKEDG	I10, 2F 10.0
4	IPR, PRM1, PRM2, NORM, NPT, N	I10, 3F 10.0, 2I10
5	UNIT, UNIT1, UNID, UNID1, NRPT, T1	A4, I6, A4, I6, I10, F 10.0
6	RS, BETAS, DS, ALPHAS	4F 10.0
7	RD, BETAD, DD, ALPHAD, A, DMAX, T	7F 10.0
8	A1, RH01, A2, RH02	4F 10.0
9	E1(1), S1(1), TLA(1), TL1(1)	4F 10.0
10	E1(2), S1(2), TLA(2), TL1(2)	4F 10.0
.	.	.
.	.	.
.	.	.

18	E1(10), S1(10), TLA(10), TL1(10)	4F 10.0
19	E2(1), S2(1), TL2(1)	4F 10.0
20	E2(2), S2(2), TL2(2)	4F 10.0
.	.	.
.	.	.
.	.	.
28	E2(10), S2(10), TL2(10)	4F 10.0
29	EBRK, EGAM	2F 10.0

If IPR = 7, the next NPT + 1 cards must each contain a single value of N with format I4, and then continue with the following string of cards.

30	SIDE(I), I = 4, 13 (omit if IPR = 8)	10A4
31	TOP(I), I = 4, 21	18A4
32	BOTTOM(I), I = 4, 21	18A4

APPENDIX E

REPRESENTATIVE RESULTS OF SIMULATION

Complete Example with Printout

INPUT LISTING SIMULATION OF AL-FE SYSTEM. COMPTON SCATTER ONLY. RUN 1.

COCE FOR PARAMETER TO BE VARIED: 5 OPTIMIZING PARAMETER: 20 TIME LIMIT, MINUTES: 19.5

RANGE: 0.0 TO 280.00

NORMALIZE TO RESPONSE AT: 0.0

NO. OF POINTS TO BE CALCULATED: 20

ASSUME UNIFORM TARGET ILLUMINATION? NO

NO. OF EVENTS AT NORMALIZING POINT: 2000

ASSUME UNIFORM DETECTOR ILLUMINATION? YES

GEOMETRY PARAMETERS

RS	0.25
BETA S	7.50
DS	8.00
ALPHAS	45.00
PD	0.25
BETA D	5.00
DD	8.00
ALPHAD	90.00
A	-1.20
D MAX	2.54
T	0.0

MATERIAL PROPERTIES

A1	55.847
RHO1	7.9
A2	26.982
RHO2	2.7

MEDIUM 1 CROSS SECTION VALUES

E	C SCAT	ABSORP	TOTAL
0.020	10.400	2050.000	2260.000
0.030	11.400	674.000	729.000
0.040	11.600	294.000	320.000
0.050	11.600	150.000	169.000
0.060	11.400	96.400	102.000
0.060	11.400	96.400	102.000
0.080	10.900	36.700	49.900
0.100	10.300	18.500	30.900
0.150	9.090	5.410	16.600
0.200	8.070	2.250	12.600

MEDIUM 2

0.030	6.230	43.600
0.040	6.250	21.200
0.050	6.170	13.800
0.060	6.030	10.600
0.090	5.690	8.010
0.050	6.170	13.800
0.060	6.030	10.600
0.080	5.690	8.010
0.100	5.360	6.990
0.150	4.650	5.350

EMPK = 0.060

EGAM = 0.100

PARAMETER 5	RESPONSE
0.0	1.000E-00
0.0	9.856E-01
1.400E 01	7.479E-01
2.800E 01	5.380E-01
4.200E 01	4.052E-01
5.600E 01	3.244E-01
7.000E 01	2.833E-01
8.400E 01	2.381E-01
9.800E 01	2.078E-01
1.120E 02	1.981E-01
1.260E 02	1.843E-01
1.400E 02	1.713E-01
1.540E 02	1.643E-01
1.680E 02	1.627E-01
1.820E 02	1.558E-01
1.960E 02	1.622E-01
2.100E 02	1.636E-01
2.240E 02	1.619E-01
2.380E 02	1.493E-01
2.520E 02	1.581E-01
2.660E 02	1.458E-01
2.800E 02	1.472E-01

Figure E-1. Al-Fe SYSTEM/100 KEV INCIDENT/COMPTON SCATTER ONLY.

Further Examples without Printout

Figure E-2. VARIATION DUE TO TRANSLATION OF THE DETECTOR.

Figure E-3. TEST OF COUNTING STATISTICS.

Figure E-4. RESPONSE AS A FUNCTION OF THE PLATING THICKNESS.

Figure E-5. OPTIMIZATION OF THE NRPT PARAMETER.