Application of DOT-MORSE Coupling to the Analysis of Three-Dimensional SNAP Shielding Problems *

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Many radiation transport problems can best be solved by using both discrete ordinates and Monte Carlo techniques with a coupling between the two techniques occurring at a geometry interface. A general discussion of two possible coupling schemes is given. The calculation of the reactor radiation scattered from a docked service and command module is used as an example of coupling discrete ordinates (DOT) and Monte Carlo (MORSE) calculations.

Many SNAP shielding problems involve determining neutron and gamma-ray transport in three-dimensional geometries. The solution of these problems by the application of Monte Carlo techniques alone frequently requires considerable computer time; however, many parts of the transport problem are only one- or two-dimensional and can easily be solved with discrete ordinates techniques. A convenient approach to solving the three-dimensional problem is to combine the discrete ordinates and Monte Carlo techniques, using Monte Carlo only for the transport that is three dimensional.

In coupling discrete ordinates with Monte Carlo, there is generally some difficulty associated with the compatibility of cross-section representation. This is due to the use of multigroup cross sections in the discrete ordinates codes and point cross sections in the Monte Carlo calculations. Additional problems in performing coupled neutron-gamma-ray calculations in the Monte Carlo part also arise in some cases. The use of the multigroup Monte Carlo code MORSE (ref. 1) alleviates both of these problems in that the same multigroup cross sections can be used in both the discrete ordinates and the Monte Carlo calculations, and the coupled neutron-gamma-ray transport can be solved as one problem.

In using the results of discrete ordinates calculations as a source term for a Monte Carlo calculation, it is desirable to use as much as possible of the detail that is available, or else determine the effect of ignoring the detail. In other words, the assumption of separation of energy, angular, and spatial variation of the radiation should be avoided.

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In general, the source term for the Monte Carlo calculation may be distributed over a volume or may be a boundary or surface source. Both types of coupling will be discussed, and then an example will be given to illustrate a specific application.

The first case to be discussed is the coupling of results of discrete ordinates calculations [in this case, DOT (ref. 2) results] to Monte Carlo with a volume or region being unique to both calculations. The results of a DOT calculation of the fluence $\Phi(r,z,E,\theta,\phi)$, a five-dimensional array defined for r,z within the volume of interest, is assumed to exist. In general, one would like to select the source term for subsequent calculations from a conditional probabilitiy distribution for particles leaving a collision as a function of each of the five variables. Because of the large array of numbers, approximations have been made in the past in which some of the variables are selected from non-conditional probabilities that are volume integrated. For example, the energy may be selected from the spectrum integrated over the volume. Likewise, the angular distribution may be assumed to be the same for all points in the volume, or for all energies. However, complete detail can be used with increased data handling and storage requirements.

The first step in coupling over a spatial region is to convert the fluence Φ to χ, the density of particles leaving a collision. This is accomplished by multiplying the fluence by the group-to-group cross section:

$$\chi(r,z,E_g,\theta,\phi) = \sum_{\theta'} \sum_{E'} \Phi(r,z,E',\theta',\phi) \times \Sigma_s(E'\rightarrow E_g,\theta'\rightarrow\theta)$$

Then, define

$$T = \sum_{v_r} 2\pi\bar{r}\Delta r \sum_{v_z} \Delta z \sum_g \sum_\ell \sum_m wt(\ell,m)\chi(r,z,E_g,\theta,\phi)$$

where $\chi(r,z,E_g,\theta,\phi)2\pi\bar{r}\Delta r\Delta z$ is defined as the density of particles leaving a collision at r,z with energy E in group g per unit polar angle θ and azimuthal angle ϕ.

$wt(\ell) = \sum_m wt(\ell,m)$ is the solid angle segment for each polar angle θ, and

$wt(\ell,m)$ = the solid angle of each azimuthal angle ϕ for each polar angle index ℓ.

In order to select from this distribution, one must form the five following distributions:

$$R(r) = \frac{2\pi\bar{r}\Delta r}{T} \sum_{v_z} \Delta z \sum_g \sum_\ell \sum_m wt(\ell,m) \times \chi(r,z,E_g,\theta,\phi) ,$$

$$Z(z|r) = \frac{2\pi\Delta z\bar{r}\Delta r}{TR(r)} \sum_g \sum_\ell \sum_m wt(\ell,m)\chi(z,E_g,\theta,\phi|r) ,$$

$$E(E|z,r) = \frac{\Delta z 2\pi\bar{r}\Delta r}{TZ(z|r)R(r)} \sum_\ell \sum_m wt(\ell,m) \times \chi(E_g,\theta,\phi|z,r) ,$$

$$P(\theta|E_g,z,r) = \frac{\Delta z 2\pi\bar{r}\Delta r}{TE(E_g|z,r)Z(z|r)R(r)} \sum_m wt(\ell,m) \times \chi(\theta,\phi|E_g,z,r) ,$$

$$A(\phi|\theta,E_g,z,r) = \frac{wt(\ell,m)\Delta z 2\pi\bar{r}\Delta r \ \chi(\phi|\theta,E,z,r)}{TP(\theta|E_g,z,r)E(E_g|z,r)Z(Z|r)R(r)} .$$

From these conditional probability distributions one may select values for the source coordinates. With the assumption of linear variation between spatial points and angular directions the discrete values are not carried forth in the Monte Carlo calculation, but instead a continuous distribution of coordinates is selected. Care must be exercised in utilizing this type of coupling so that the transport in the overlap region is not included twice. This may be accomplished using a pure absorber in the overlap region in the Monte Carlo calculation.

Perhaps a more useful coupling technique is the coupling at a boundary of the system. For this case, similar conditional probabilities must also be formed, with some minor exceptions. Consider the coupling surface to be the outer boundary of a cylinder.

The leakage fluence, $\Phi(r,Z,E_g,\theta,\phi)$, at the top, bottom, and curved surface of a cylinder is determined as a function of energy, polar, and azimuthal angles, as well as the spatial variation on the surfaces. The leakage fluence on these surfaces designated as R_o, Z_T, and Z_B must be converted to current for the selection of the source term of the Monte Carlo calculation. Thus, there are three spatial terms - the radial variation at the top, the radial variation at the bottom, and the height variation at the outer surface of the cylinder. Define T, B, and S for the integrated leakage for the top, bottom, and side of the cylinder.

$$T = \sum_{0,R_o} 2\pi\bar{r}\Delta r \sum_{E_g} \sum_{\cos\theta>0} \cos(\theta_\ell)\sum_m wt(\ell,m) \times \Phi(r,Z_T,E_g,\theta,\phi) ,$$

$$B = \sum_{0,R_o} 2\pi\bar{r}\Delta r \sum_{E_g} \sum_{\cos\theta<0} |\cos(\theta_\ell)| \times \sum_m wt(\ell,m)\Phi(r,Z_B,E_g,\theta,\phi) ,$$

$$S = 2\pi R_o \sum_{Z_B,Z_T} \Delta z \sum_{E_g} \sum_\ell \sin(\theta_\ell) \sum_{\cos\phi>0} \times wt(\ell,m)\cos\phi \ \Phi(R_o,Z,E_g,\theta,\phi) ,$$

with total leakage TL = T + B + S.

For each of the above terms, a four-dimensional conditional probability must be determined. For example, consider the bottom surface leakage:

$$R_B(r) = \frac{2\pi\bar{r}\Delta r}{B} \sum_{E_g} \sum_{\cos\theta<0} |\cos(\theta)| \sum_m \times wt(\ell,m)\Phi(r,Z_B,E_g,\theta,\phi) ,$$

$$E_B(E_g|r) = \frac{2\pi\bar{r}\Delta r}{BR(r)} \sum_{\cos\theta<0} |\cos(\theta)| \sum_m wt(\ell,m) \times \Phi(r,Z_B,E_g,\theta,\phi) ,$$

$$P_B(\theta|E_g,r) = \frac{2\pi\bar{r}\Delta r|\cos(\theta)|}{BR(r)E_B(E_g|r)} \sum_m wt(\ell,m) \times \phi(r,Z_B,E_g,\theta,\phi) ,$$

$$A_B(\phi|\theta,E_g,r) = \frac{2\pi\bar{r}\Delta r|\cos\theta|wt(\ell,m)}{BR(r)E_B(E_g|r)P_B(\theta|E_g,r)} \times \phi(r,Z_B,E_g,\theta,\phi) .$$

The results for the top surface leakage and side leakage are similar.

With probability B/TL and T/TL the source would be selected from the bottom and top surface, respectively, and with probability S/TL the source would be selected from the side of the cylinder. Then, given the spatial coordinates, an energy group is chosen from E_B, and then the direction cosines are chosen for P_B and A_B.

The selection from the probability distribution given above is sometimes hindered by negative fluxes in the DOT-calculated source term. If there are no negative values, then the selection of a value x is selected from the distribution by choosing a random number R and finding j such that

$$\sum_{k=0}^{j-1} P(x_k) < R \leq \sum_{k=0}^{j} P(x_k);$$

then

$$x = \frac{[R - P(x_{j-1})]}{P(x_j) - P(x_{j-1})} (x_j - x_{j-1}) + x_{j-1} .$$

However, if some values of the distribution $P(x_j)$ are negative, then an alternate scheme is required. The random number is scaled by the sum of the absolute values of the probabilities and a selection is made. A weight correction is required which can result in negative particle weights. These negative weights in general will not severely affect the solution, but they do, of course, affect the variance of the result.

$$\sum_{k=0}^{j-1} |P(x_k)| < R*SUM \leq \sum_{k=0}^{j} |P(x_k)| ,$$

where

$$SUM = \sum_{k=0}^{Nk} |P(x_k)|$$

and

$$wate = wate* \frac{P(x_j)}{|P(x_j)|} *SUM .$$

If there is a large probability of selecting a negative weight, then the DOT source term should be recalculated.

To illustrate DOT-MORSE coupling, we have considered a problem in which the coupling is at a boundary surface. More specifically, the problem consists of calculating the radiation scattered from a docked command and service module due to the leakage radiation from a 600-kWt ZrH reactor (with its associated shielding). The problem is illustrated in figure 1. The problem which consists of determining the scattered neutron and gamma-ray dose at a detector plane due to neutrons and gamma rays leaking from the reactor power assembly has previously been investigated at Atomics International (refs. 3 and 4). A drawing of the reactor and shield assembly is shown in figure 2.

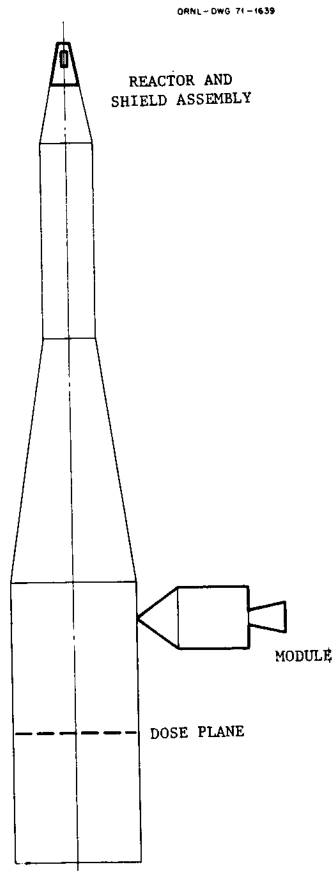

FIGURE 1.-Schematic of Reactor Power System and Docked Service and Command Module.

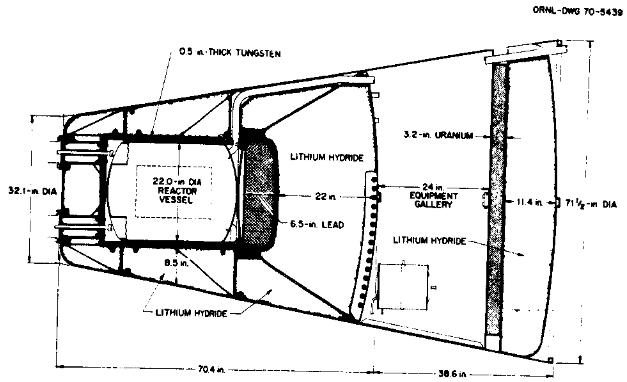

FIGURE 2.-Reactor Shield Assembly.

There are several approaches that could be used in determining the dose due to radiation scattering from the docked module. For example, one may use the boundary leakage flux obtained in a discrete ordinates calculation of the reactor and shield assembly as a source term for the Monte Carlo calculation, transport the radiation to the module, follow the transport in the service module, and estimate the dose at the detector plane. A second approach is to perform an adjoint calculation of the importance of radiation leaking from the core-shield assembly by Monte Carlo and then integrate the importance function over the source of particles leaking from the reactor assembly which was obtained in a discrete ordinates calculation. Another approach is to determine the spatial and energy distribution of the fluence at a surface surrounding the module and use this surface as the boundary for coupling the discrete ordinates results to a Monte Carlo calculation of the scattering in the service module. This last approach will be discussed.

A two-dimensional calculation of the reactor and shield assembly, as shown in figure 2, was made with the DOT (ref. 2) code. An S_8 quadrature was used to determine the energy spectra in 21 neutron and 18 gamma-ray groups. The radiation field at 15 radial locations along a plane at the top of the service module was obtained with SPACETRAN (ref. 2) using the leakage boundary fluence. SPACETRAN performs a ray-tracing calculation from each spatial mesh point to the detector point. The intensity and energy distribution of both neutrons and gamma rays was determined for each of these 15 locations. See Table I for energy group structure and fluence-to-dose conversion factors. The angular distribution of the source was determined by assuming that all the radiation was coming from the center of the reactor core located approximately 90 feet away. (The problem is not expected to be very sensitive to the small angular variation of the radiation incident on the module.) This radiation field as a function of space and energy was used as the source term for Monte Carlo.

Table I. Energy Group Structure and Fluence-To-Dose Conversion Factors

Group	Upper Energy (eV)	Fluence-to-Dose Conversion Factors (mrem/hr)/ (part/cm^2/sec)
Neutrons:		
1	1.4918(+7)*	1.5000(-1)
2	1.0000(+7)	1.5000(-1)
3	6.7032(+6)	1.3700(-1)
4	4.4933(+6)	1.3200(-1)
5	3.0119(+6)	1.3100(-1)
6	2.0190(+6)	1.2500(-1)
7	1.3534(+6)	1.1600(-1)
8	9.0718(+5)	1.0600(-1)
9	5.5023(+5)	7.5700(-2)
10	3.3373(+5)	5.5100(-2)
11	2.0242(+5)	4.0100(-2)
12	1.2277(+5)	2.4500(-2)
13	4.0867(+4)	8.5000(-3)
14	1.1709(+4)	5.0000(-3)
15	3.3546(+3)	5.0000(-3)
16	7.4852(+2)	5.0000(-3)
17	1.6702(+2)	5.0000(-3)
18	3.7266(+1)	5.0000(-3)
19	8.3153(0)	5.0000(-3)
20	1.8554(0)	5.0000(-3)
21	4.1399(-1)	3.7500(-3)
Gamma Rays:		
22	1.0000(+7)	9.8000(-3)
23	8.0000(+6)	8.5000(-3)
24	7.0000(+6)	7.6000(-3)
25	6.0000(+6)	6.7000(-3)
26	5.0000(+6)	5.8000(-3)
27	4.0000(+6)	5.0000(-3)
28	3.5000(+6)	4.5000(-3)
29	3.0000(+6)	4.0000(-3)
30	2.5000(+6)	3.5000(-3)
31	2.0000(+6)	3.0000(-3)
32	1.6000(+6)	2.4000(-3)
33	1.2000(+6)	2.0000(-3)
34	9.0000(+5)	1.5000(-3)
35	6.0000(+5)	1.0500(-3)
36	4.0000(+5)	6.0000(-4)
37	2.1000(+5)	2.8000(-4)
38	1.2000(+5)	1.4000(-4)
39	7.0000(+4)	4.0000(-4)

*Read as 1.4918×10^7.

At a plane just above the module, the intensity variation was determined to be that shown in figure 3. The energy distribution, or the number in each of the 21 neutron groups and 18 gamma-ray groups, is shown as a cumulative distribution for three different radii in figure 4. These curves illustrate the distributions used for the selection of the source in the MORSE Monte Carlo calculation. By using MORSE, it was possible to determine the contribution to the scattered dose of the incident neutrons and gamma rays as well as the secondary gamma rays produced in the module.

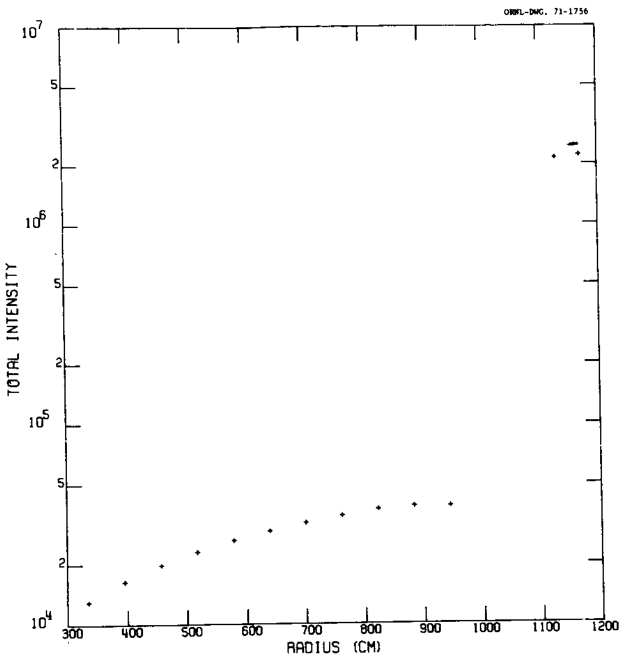

FIGURE 3.-Spatial Distribution of Radiation at Source Plane Adjacent to the Service and Command Module.

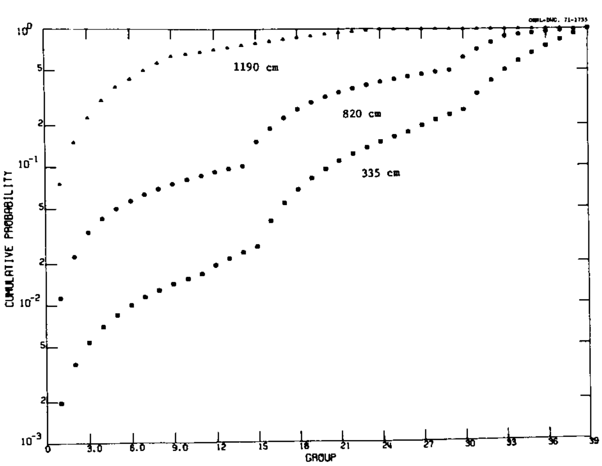

FIGURE 4.-Cumulative Probability for Energy Distribution of Neutrons and Gamma Rays at Three Locations Along Source Plane.

The geometry employed in the calculation is illustrated in figure 5, which shows boundary crossing events in the transport of neutrons in the module. The radial and longitudinal location of the crossing events is shown. This collision density plot is an output from MORSE and gives the boundary crossings for approximately 1000 source particles. The typed numbers give the density of the homogenized parts of the service module, and Table II gives the material composition for each region. Figure 6 shows the density of collisions of neutrons in one particular problem. The rotational symmetry of the module is taken into account in the plot, and there are few collisions in the center. The use of this type of on-line plot has been useful in determining where the events are occurring and the effects of importance sampling.

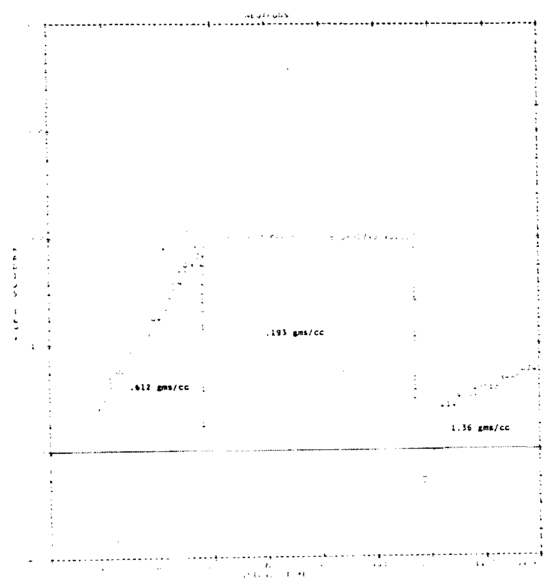

FIGURE 5.-Boundary Crossing Events From a MORSE Calculation. The density of the three material regions is given.

Table II. Material Composition for the Service and Command Module

Medium	Weight (lbs)	Density (gm/cc)	Composition (wt %)				
			H	O	Al	Ti	Fe
1	13,500	0.612	3.3	46.7	20.0	17.0	13.0
2	20,800	0.193	3.3	46.7	20.0	17.0	13.0
3	200	1.36					100.0

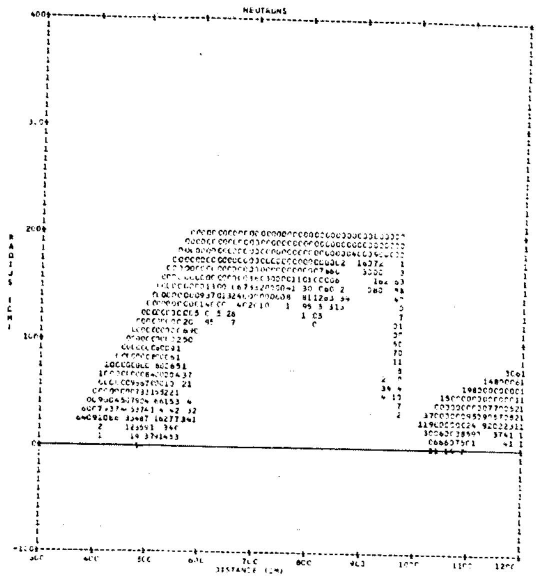

FIGURE 6.-Collision Density Plot for Neutrons Scattering in the Service and Command Module. Numbers 1-9 include the number of collisions in the intervals with 0 indicating 10 or more collisions.

The contribution of scattered neutrons and gamma rays to the dose at the detector plane (117 ft from the reactor) is shown in Table III (about 5% of the gamma-ray dose is due to secondary gamma rays produced in the service module). The total scattered dose of 0.34 mrem/hr should be compared to the direct dose of 0.70 mrem/hr (0.66 mrem/hr gamma rays and 0.04 mrem/hr neutrons). These results are compared with values calculated at Atomics International for various locations on the detector plane. There is surprisingly good agreement between the Monte Carlo and single-scattering results.

Table III. Scattered Dose at the Detector Plane (mrem/hr)

Detector Location (ft)		Neutron Dose		Gamma-Ray Dose		Total	
Along Axis	⊥ Axis	Single Scattering*	Monte Carlo	Single Scattering	Monte Carlo	Single Scattering	Monte Carlo
0	0	0.228	0.29	0.063	0.05	0.30	0.34
11	0	0.73	0.31	0.27	0.08	1.0	0.39
0	11	0.27	0.39	0.09	0.04	0.36	0.43

*With self-absorption.

As a check on the adequacy of the SPACETRAN calculated spatial distribution at the service module location, a DOT calculation with a 100-angle quadrature biased in the downward direction was made. Figures 7 and 8 show the spatial distribution at the source plane and the energy distributions. There are fairly large differences in these results compared to those in figures 3 and 4 ; however, the scattered dose contribution does not change more than 15%.

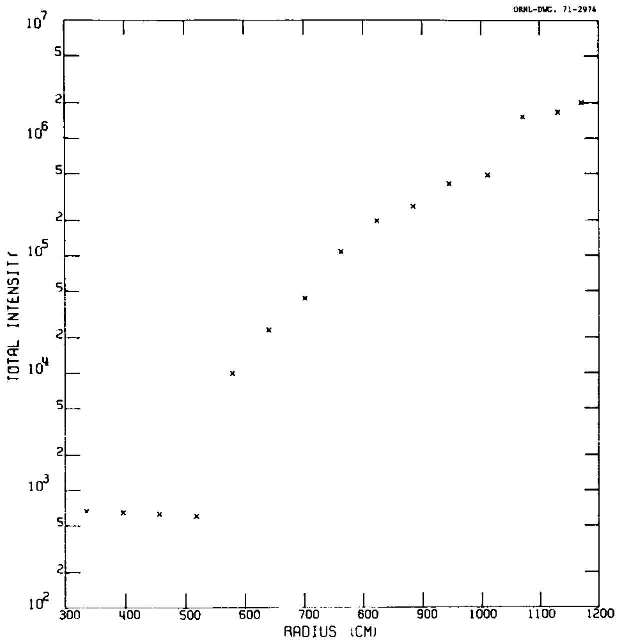

FIGURE 7.-Spatial Distribution of Radiation at Source Plane Adjacent to the Service and Command Module Calculated With a 100-angle Asymmetric Quadrature.

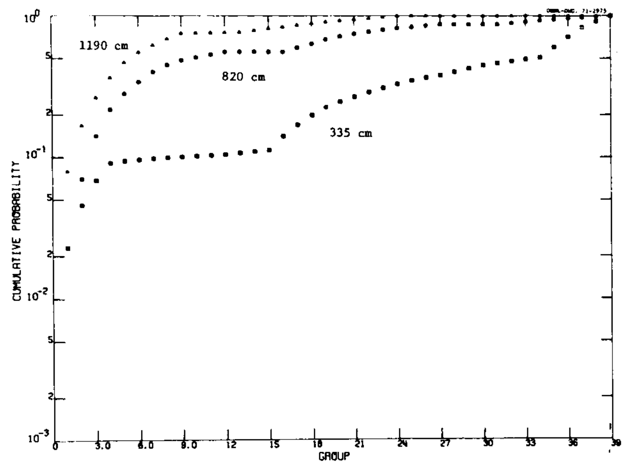

FIGURE 8.-Cumulative Probability for Energy Distribution of Neutrons and Gamma Rays at Three Locations Along Source Plane Calculated With a 100-angle Asymmetric Quadrature.

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