Discrete Ordinates - Monte Carlo Coupling: A Comparison of Techniques in NERVA Radiation Analysis*

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In the radiation analysis of the NERVA Nuclear Rocket System, two-dimensional discrete ordinates calculations are sufficient to provide detail in the pressure vessel and reactor assembly. Other parts of the system, however, require three-dimensional Monte Carlo analyses. To use these two methods in a single analysis, a means of coupling was developed whereby the results of a discrete ordinates calculation can be used to produce source data for a Monte Carlo calculation. Several techniques for producing source detail were investigated. Results of calculations on the NERVA system are compared and limitations and advantages of the coupling techniques discussed.

In the analysis of the NERVA** nuclear rocket engine, a complex radiation transport problem must be solved. Since any shield design must simultaneously minimize weight and radiation level, both penetration and geometry effects are important.

ANALYSIS METHODS

Two rigorous methods have found wide application in complex radiation transport problems: discrete ordinates (S_N) and Monte Carlo. A wide range of computer codes is available for both methods.

The discrete ordinates (S_N) method can be used in one-dimensional or two-dimensional problems. It employs an iterative balance of radiation in a large number of mesh regions. Angular and energy dependence is calculated in a limited number of preselected directions and energy groups. Collision angle-to-angle and energy-to-energy transfers are determined by expansions of the scattering probability in terms of Legendre polynomials. Where these approximations can be employed, the method allows a relatively rapid evaluation of radiation transport throughout a system. If the system contains voids or regions of widely varying collision densities, two-dimensional analyses may result in anomalies called ray effects(1) in which the allowed directions do not properly intercept regions of interest. No three-dimensional representation is possible.

The Monte Carlo method may allow pointwise representation of radiation distribution in space, energy, and angle with exact kinematics to the degree to which cross section data are available. Any amount of detail must be paid for in computer time. The Monte Carlo method calculates and tabulates the fates of individual particles (or individual "particles" which may represent any number of real particles or energy quanta). If relatively few collisions occur or averages over large regions, angles, or energies are allowed, the method can be quite efficient.

APPLICATION TO NERVA

A NERVA propulsion module consists of a propellant tank and engine which includes pressure vessel and reactor assembly, shielding, nozzle, and the necessary pumps, pipes, valves, instrumentation, and controls. A typical layout is shown in Figure 1.

The pressure vessel and reactor assembly (PVARA) is the primary source of radiation. For radiation analysis purposes, it consists of a core, beryllium reflector, forward internal shield, and pressure vessel. The PVARA is essentially a two-dimensional object and can be accurately modeled in cylindrical geometry. The PVARA materials are sufficiently dense so that many mean free paths would be seen by particles before leaking from the outer surfaces of the pressure vessel. Pure analog Monte Carlo analyses of the PVARA would be very costly in computer time, especially if statistically valid radiation leakage data are needed in narrow bands of space, angle, or energy.

The portion of the engine between the PVARA and the propellant tank includes several thousand pounds of metallic components in complicated three-dimensional geometries with many void regions. In the nearly empty condition, the propellant tank and

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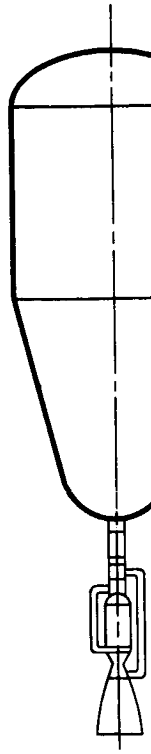

Figure 1

NUCLEAR PROPULSION MODULE CONFIGURATION

liquid hydrogen impose few mean free paths to most radiation.

A comparison of the capacities of the analytical methods and the characteristics of the system indicates that Monte Carlo is necessary for most regions but S_N may be sufficient for analysis of the pressure vessel and reactor assembly.

METHOD COUPLING

If S_N were to be used for analysis of the PVARA and Monte Carlo for most other regions of the system, a means must be devised for producing source information for Monte Carlo from S_N results. This information must be in sufficient detail for the needs of any desired analysis.

In each spatial mesh in each energy group, an angular flux can be calculated by S_N along several predetermined vectors. Each such vector can be visualized as a line from the center of an igloo to the center of a block of the igloo. Figure 2 indicates how such an igloo would describe the directions in which the angular flux could be described in a single radial band on the top surface of the reactor cylinder. The S_N fluxes are tabulated in energy, space, and angle. One could define a "particle" for each such vector in terms of the particles/second value of the tabulated flux. These vectors, if continued by Monte Carlo through a void or low density region, would not necessarily intersect regions of interest. This is comparable to the "ray effects" obtained if the S_N model contains voids. To more nearly represent the physical problem, the particle directions must be distributed uniformly over that part of the igloo that can be seen from the regions of interest.

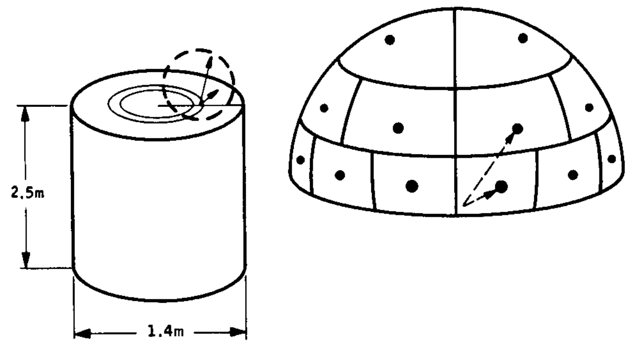

Figure 2

S_N ANGULAR DESCRIPTION

HISTOGRAM

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

SMOOTHING

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

TAILORED QUADRATURES

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

COMPARISON OF METHODS

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

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

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

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

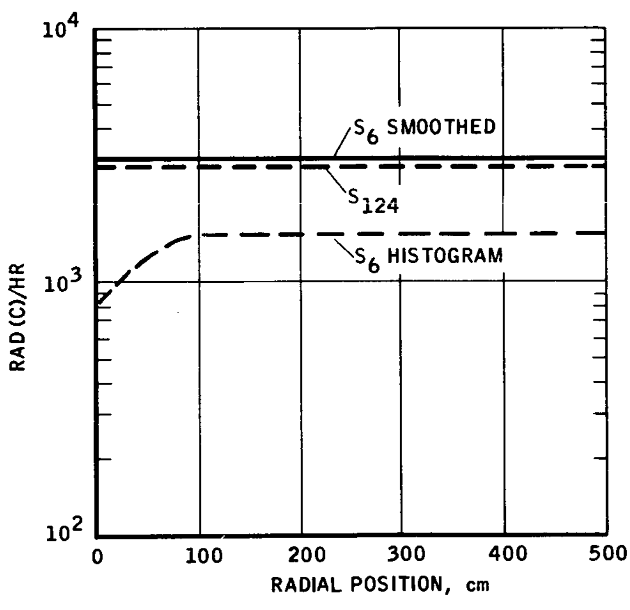

Figure 3

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

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

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

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

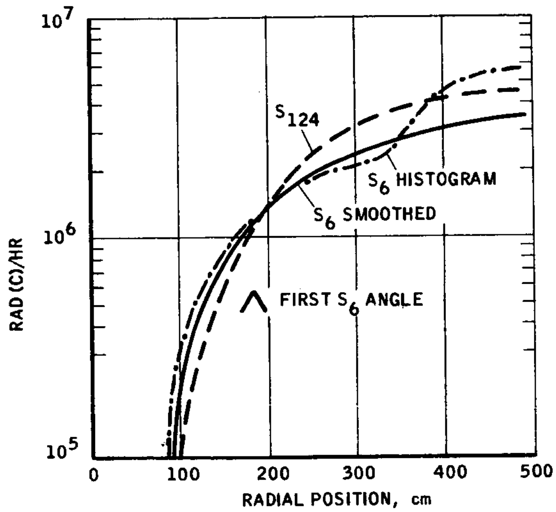

Figure 4

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

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

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

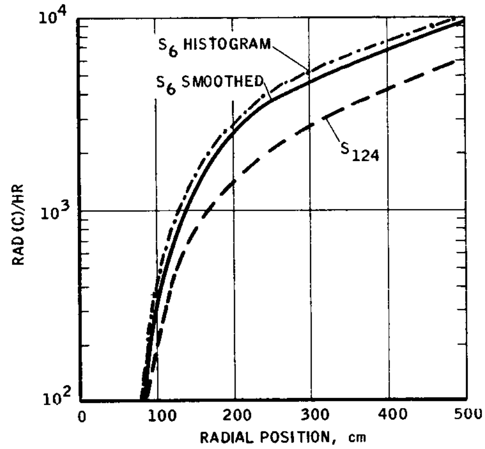

Figure 5

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

COUPLING INTERNAL TO THE S_N PROBLEM

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

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

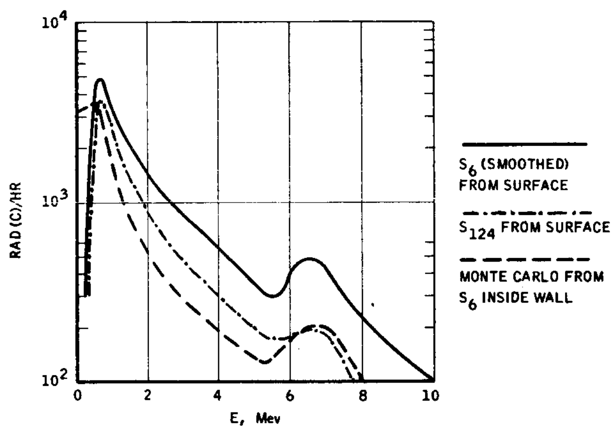

Figure 6

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

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

In a similar application, an S_6 DOT calculation was used to produce angular flux information between the reactor core and reflector. The particles simulated at this interface were traced through the reflector and wall regions by COHORT to a surface above the reactor, and a data tape of particle information produced. A pure Monte Carlo calculation of sources in the reflector and wall was also run using COHORT to produce a second data tape of particle information above the reactor. These data tapes were then used with a COHORT model of a propellant tank to calculate radiation levels at the top of the tank with different quantities of liquid hydrogen in the tank.

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

OTHER EXAMPLES OF THE METHOD OF CODE COUPLING

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

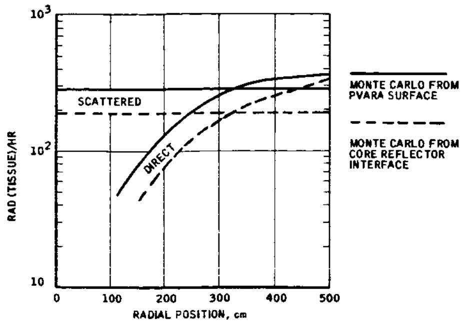

Figure 7

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

ADVANTAGES OF THE METHOD OF CODE COUPLING

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

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

But many scatters are necessary in the wall. Probably this problem would be prohibitively costly in computer time for all but the most liberally financed establishments. Using the S_N - Monte Carlo coupling technique, however, the problem can be quite economical. A low quadrature S_N can be run on an IBM 360/65 in an hour or less for a 10 - 20 energy group, 50 x 30 spatial mesh problem. A high quadrature problem, such as an S_{124}, may take two to three times as long. The DASH problem to produce Monte Carlo data or calculate transport through a void or pure absorber takes 5 to 10 minutes. DASH can produce any required number of source particles. A Monte Carlo problem in the wall would take a few minutes longer. The whole process takes little more time than the original S_N. Furthermore, once the S_N problem has been run and the angular flux data saved on magnetic tape, it can be used any number of times. This allows additional analyses tailored to specific needs at any later time without repeating the bulk of the calculations. Later calculations can be performed in any degree of Monte Carlo employment, from pure S_N to pure Monte Carlo, with commensurate computer costs.

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

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