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APPLICATION OF ADJOINT DIFFERENCE AND SURFACE INTEGRAL METHODS TO SELECTED DEEP-PENETRATION RADIATION TRANSPORT PROBLEMS

Final Report

Prepared by

The University of Tennessee
Knoxville, Tennessee

and

Oak Ridge National Laboratory
Oak Ridge, Tennessee

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The theoretical considerations lead to the conclusion that an error is associated with the Surface Integral technique, but this error will probably be small for the class of problems considered herein. In contrast to this, the Adjoint Difference technique is "exact". The numerical results presented agree with these predictions.

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FINAL REPORT

J. C. Robinson
P. N. Stevens

THE UNIVERSITY OF TENNESSEE
Knoxville, Tennessee

T. J. Hoffman

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee

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The theoretical considerations lead to the conclusion that an error is associated with the Surface Integral technique, but this error will probably be small for the class of problems considered herein. In contrast to this, the Adjoint Difference technique is "exact". The numerical results presented agree with these predictions.

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I. INTRODUCTION

The objective of this project was to develop efficient calculational techniques to predict the absorbed radiation within geometrically complex targets, e.g. re-entry vehicles. The targets are normally far removed from the source responsible for the radiation field; therefore the overall problem can be described as a geometrically complex deep penetration problem.

In this study, it was assumed (for convenience) that the target was located in air or at an air-ground interface. The overall problem was broken up into three separate steps:

1. The calculation of the free field radiation (deep penetration problem) in the air (or air-ground interface) with the target absent.
2. The calculations associated with the geometrically complex target without explicitly accounting for the source.
3. The combination of the results from the first two steps to obtain the quantity of interest for a particular source-target geometric configuration.

The first step can be described as a deep penetration problem, which is geometrically simple (one or two-dimensional). Accordingly, this problem was solved using deterministic techniques, i.e., the discrete ordinate codes ANISN[1] and DOT[2]. The second step is a geometrically complex problem, but usually not one of deep penetration. Hence, rather straightforward Monte Carlo techniques are well suited for the calculational tool. The code MORSE[3] was used here. A code was written

to implement the third step for demonstrative purposes. This implementation of this last step of the overall procedure becomes somewhat involved for arbitrary orientations of the target relative to the source. The complications are introduced by the fact that the reference coordinate system used for the calculations associated with step one are different than the reference coordinate system used for step 2.

The calculation procedures employed require the solutions to the forward neutron transport equation for step one and the adjoint transport equation for step 2. The adjoint transport equation was solved with two different sets of boundary conditions resulting in two different ways of obtaining the quantity of interest, i.e., the Surface Integral Approximation technique and the Adjoint Difference technique. Each of these methods will be presented below.

The theoretical development and the associated computational procedures for both the Surface Integral Approximation and Adjoint Difference techniques are reported in detail in a doctoral dissertation which was completed in connection with this project and reported in Ref. 4. Furthermore, sufficient examples are included in Ref. 4 to demonstrate the applicability of each technique. This report will include only the more important aspects of the theoretical results. The reader interested in the more detailed development and implementation is referred to Ref 4 (R-4). For completeness, the results of all test problems which have been considered will be included in this report (some of these are also presented in R-4).

II. THEORETICAL CONSIDERATIONS

A. Introduction

In this section, the problem of computing the effect of interest within a target removed from the source responsible for the radiation field is considered. The formulation is presented so that the effect of interest can be obtained by the three distinct steps outlined in the preceeding section using both the Surface Integral and the Adjoint Difference techniques. The development here is kept brief since the more detailed development is presented in R-4.

B. Problem Statement

Let λ be the effect of interest and $R(\bar{p})$ be the response function (i.e., the contribution to λ due to unit angular flux), then the problem is to solve the integral equation

$$\lambda = \int \phi_1(\bar{p}) R(\bar{p}) d\bar{p} \tag{1}$$

where $\phi_1(\bar{p})$ is the angular flux. The angular flux is the solution to the Boltzmann transport equation

$$H_1(\bar{p})\phi_1(\bar{p}) = S(\bar{p}), \tag{2}$$

where $S(\bar{p})$ is the source, $H_1(\bar{p})$ is the integro-differential operator of the Boltzmann equation (see R-4), and subscript "1" refers to the medium with the target located in air.

C. The Surface Integral Approximation

For the Surface Integral method, a closed surface, denoted by $\bar{r}_s$, is selected apriori which encloses the target and excludes the source.

Then the effect of interest can be obtained by solving the integral equation

$$\lambda = - \int_{\bar{p}_1} (\bar{\Omega}\cdot\bar{n})_{in}\delta(\bar{r}-\bar{r}_s)\ \phi_1(\bar{p})\phi^*(\bar{p})d\bar{p}. \tag{3}$$

In Eq. 3, $\bar{p}_1$ represents the phase space interior to the surface $\bar{r}_s$, $\bar{n}$ is the outward directed normal to the surface $\bar{r}_s$, the subscript "in" represents inward directed $\bar{\Omega}$ only, and $\phi^*(\bar{p})$ is the solution to

$$H_1^*\ (\bar{p})\ \phi^*(\bar{p}) = R(\bar{p}). \tag{4}$$

In Eq. 4, $H_1^*(\bar{p})$ is the operator adjoint to the operator $H_1(\bar{p})$ of Eq. 2, and the boundary condition is

$$\phi^*(\bar{p}) = 0 \tag{5}$$

for $(\bar{n}\cdot\bar{\Omega}) > 0$ at the surface $\bar{r}_s$.

There are no approximations associated with Eq. 3, but this formulation for the effect of interest is of little practical value since it is still necessary to solve Eq. 2 for $\phi_1(\bar{p})$. However, we need $\phi_1(\bar{p})$ at the surface $\bar{r}_s$ for inward directions only.

To introduce the Surface Integral Approximation, consider the solution to

$$H_2(\bar{p})\ \phi_2(\bar{p}) = S(\bar{p}), \tag{6}$$

where $H_2(\bar{p})$ is the integro-differential operator of the Boltzmann equation, $S(\bar{p})$ is the same source as in Eq. 2, and subscript 2 refers to the medium with the target removed. Assume that the $\phi_1(\bar{p})$ of Eq. 3 can be adequately approximated with $\phi_2(\bar{p})$*, then

---

*We are assuming the inward directed component of the flux at the surface $\bar{r}_s$ is uneffected by the presence of the vehicle.

$$\lambda = - \int_{\bar{p}_1} (\bar{\Omega}\cdot\bar{n})_{in}\ \delta(\bar{r}-\bar{r}_s)\ \phi_2(\bar{p})\ \phi^*(\bar{p})d\bar{p} \tag{7}$$

which is the Surface Integral Approximation.

To summarize, the Surface Integral Approximation consists of the following steps:

1. Calculation of the free field radiation in the medium (air) with the target absent, i.e., solution to Eq. 6.
2. Calculation of $\phi^*(\bar{p})$ (solution to Eq. 4) with boundary conditions given by Eq. 5.
3. Carry out the indicated surface integration of Eq. 7.

The relative location of the source to the target is accounted for in Step 3; therefore, many relative locations of the source and target can be analysized by a single completion of steps 1 and 2 and repeated application of step 3.

D. The Adjoint Difference Method

For the adjoint difference formulation we introduce the difference flux, $\psi(\bar{p})$, as

$$\psi(\bar{p}) \equiv \phi_2(\bar{p}) - \phi_1(\bar{p}), \tag{8}$$

where $\phi_2(\bar{p})$ is as defined in Eq. 6 and $\phi_1(\bar{p})$ is as defined in Eq. 2. The Boltzmann equation for the difference flux (using Eqs. 2, 6, and 8) is found to be

$$H_1(\bar{p})\ \psi(\bar{p}) = f(\bar{p}), \tag{9}$$

where

$$f(\bar{p}) \equiv [H_1(\bar{p}) - H_2(\bar{p})]\ \phi_2(\bar{p}). \tag{10}$$

Assume $\phi_2(\bar{p})$ throughout all phase space is known, then $f(\bar{p})$ can be considered as a source which is non zero only in the region occupied

by the vehicle. Introducing the adjoint difference flux $\psi^*(\bar{p})$, the effect of interest can be obtained from

$$\lambda = \int \phi_2(\bar{p})R(\bar{p})d\bar{p} - \int \psi^*(\bar{p})f(\bar{p})d\bar{p}, \tag{11}$$

where no approximations have been introduced. In Eq. 11, the adjoint flux is the solution to*

$$H_1^*(\bar{p})\ \psi^*(\bar{p}) = R(\bar{p}) \tag{12}$$

with the physical boundary condition that $\psi^*(\bar{p})$ for $(\bar{n}\cdot\bar{\Omega}) > 0$ goes to zero at infinity (or the physical boundary of the system).

As in the Surface Integral Approximation technique, the Adjoint Difference technique requires the solution to the free field radiation problem (solution to Eq. 6) and the adjoint function which is the solution to Eq. 12. Then the effect of interest is obtained by solving Eq. 11. The relative source-target locations are accounted for in the solution of Eq. 11.

---

*Eq. 12 differs from Eq. 4 only in the imposed boundary conditions on the dependent variable. If the same boundary conditions are imposed, it is shown in R.4 that the effect of interest from Eqs. 7 and 11 are mathematically equivalent.

III. RESULTS FOR NONFISSILE PROBLEMS

A. Introduction

A total of seven test problems which do not contain fissile materials have been considered. The first three of these seven problems can be treated as one-dimensional; therefore, the results obtained for these one dimensional problems from the Surface Integral and Adjoint Difference techniques are compared with more conventional techniques. The next three problems are geometrically more complex; hence only the results from the Surface Integral and Adjoint Difference techniques are presented. The first six problems all involve a target located in an infinite air medium, but the seventh problem involves a target (perturbing region) located in air at the air-ground interface. Accordingly, the forward flux (the unperturbed flux) for the first six problems was obtained using the one-dimensional discrete ordinates code ANISN[1], and the forward flux for the seventh problem was obtained using the two-dimensional code DOT.[2]

Results obtained from several techniques will be presented; therefore, the next section is included for the purpose of clarifying the nomenclature used in the presentation of the results. Following the establishment of the nomenclature, the results obtained for the seven problems will be presented in the order in which they were considered.

B. Nomenclature

In every case, the objective was to obtain an effect of interest, λ, as given by Eq. 1. In some problems, Eq. 2 was solved directly

using the discrete ordinates code ANISN[1] and then solving Eq. 1. Results obtained in this manner will be classified as the "ANISN method."

A second direct approach is to solve Eq. 4 (the adjoint flux) for the overall problem. Then

$$\lambda = \int_{\bar{p}} \phi^*(\bar{p})\, S(\bar{p})\, d\bar{p}. \tag{13}$$

The adjoint equations are solved using Monte Carlo techniques; therefore, results obtained this way are classified as the "Adjoint Monte Carlo method." The ANISN and Adjoint Monte Carlo methods are both well established techniques; hence results obtained this way are accepted as the correct results.

The use of Eq. 3 for the estimation of λ is classified as the "Surface Integral method." The more practical but approximate estimate of λ from Eq. 7 is the "Surface Integral Approximate method."

The use of Eq. 11 for the evaluation of λ is the "Adjoint Difference method." Finally, the use of the $\phi^*(\bar{p})$ of Eq. 4 in Eq. 11 in place of $\psi^*(\bar{p})$ leads to the "Adjoint Difference Approximate method."

C. Problems 1, 2, and 3

The first three problems were selected to demonstrate the validity and utility of the surface integral and adjoint difference formulations. Accordingly, problems are considered which could be analysized with the more standard procedures.

<u>Description of Problem 1, 2, and 3.</u> For each problem, the unperturbed problem consists of a point fission-spectrum neutron source located in an infinite air medium. Since the average mean free path

of a fission neutron in air is 86.5 meters, the unperturbed flux is assumed spatially constant over all perturbing regions. The multigroup transport equations are used as the analytic model. The group constants are those normally used for air transport problems using the codes ANISN[1] or DOT[2] by the Neutron Physics Division of the Oak Ridge National Laboratory. For the results presented in this report, all ANISN calculations were performed using either S_4 or S_{16} angular quadratures for the flux.

For Problem 1, the perturbation consisted of two concentric spherical shells or iron (2 cm. thick) with a 6 cm. air gap between the iron shells. The quantity of interest was assumed to be the response of a detector (specified below) located at the midpoint of the air gap enclosed by the spherical shells. The detector is 1000 m from the point source. The geometric details are presented in Fig. 1.

Problem 2 was identical to Problem 1 with the exception that the air gap enclosed by the spherical shells was filled with water.

Problem 3 consists of a 2 cm. thick iron spherical shell with an outside diameter of 10 cm. The shell is filled with water. A point fast flux detector is located at the center of the spherical shell. The problem is to compute the detector response at specified distances, R, from the point fission source. The geometric configuration is shown in Fig. 2.

<u>Results for Problems 1, 2, and 3.</u> The results for Problem 1 are presented in Table 1. The computed detector response is the total fast flux for the first 13 energy groups (E>0.111 Mev).

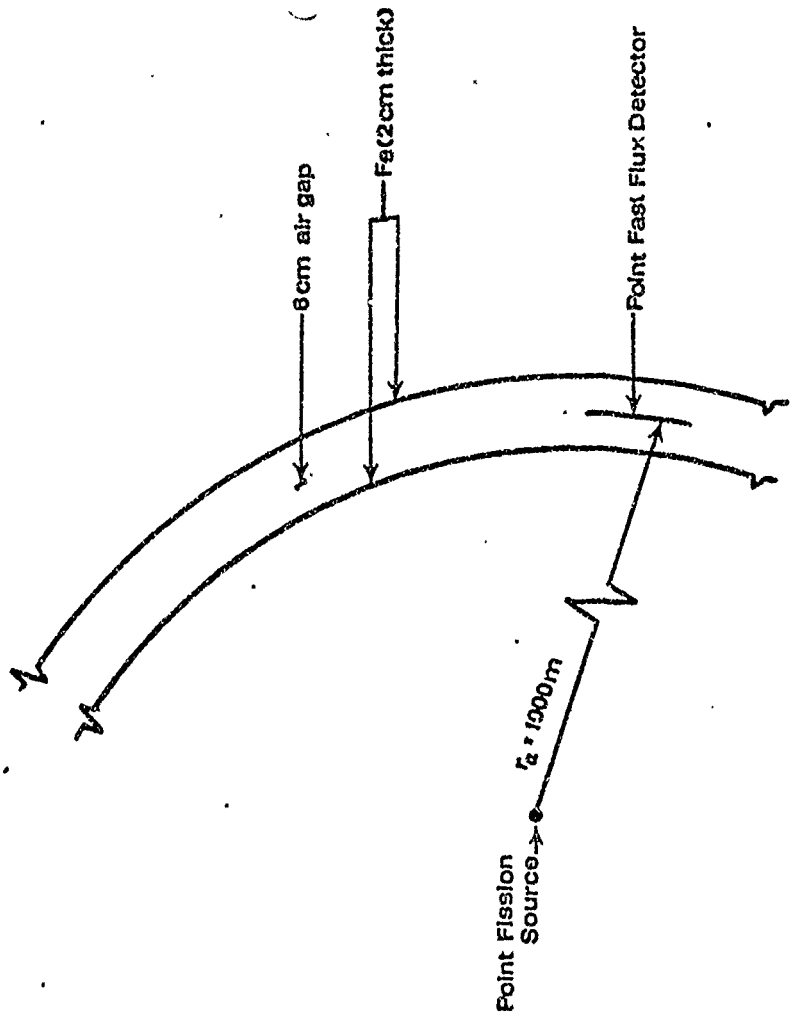

Figure 1: Geometric Configuration for Problem 1.

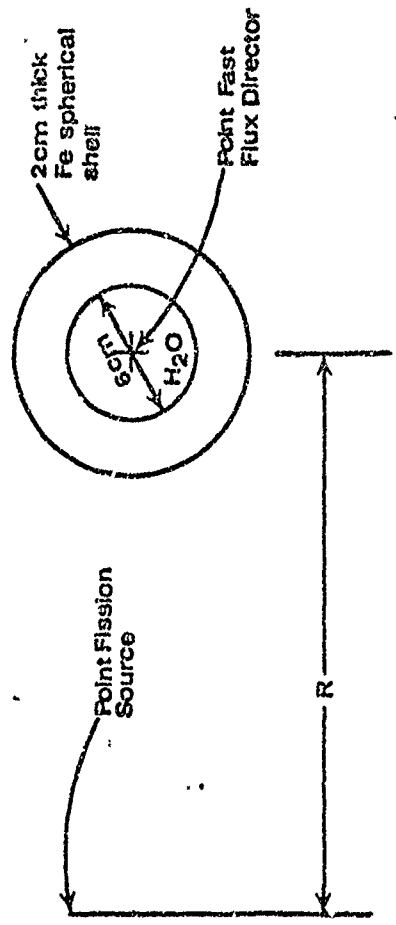

Figure 2: Geometric Configuration for Problem 3.

TABLE I

RESULTS FOR PROBLEM I

METHOD	HISTORIES	FLUENCY	COMMENTS
ANISN	———	7.13×10^{-13}	S_4 A
Adj. Diff.	4000	6.95×10^{-13}	S_4 ANISN calc.
Surf. Int.	4000	6.98×10^{-13}	
Surf. Int. Approx.	4000	7.15×10^{-13}	

The results for problem 2 are presented in Table 2.

The results, total fast flux for the first 13 groups, for Problem 3 are presented in Table 3. The parameter R is the distance from the source to the detector, see Fig. 2. The surface over which the integrations were carried out for the Surface Integral Approximation method was the Fe-air interface surface.

Discussion of Results for Problems 1, 2, and 3. From the results from the ANISN, Adjoint Difference, and Surface Integral methods for problem 1 and 2 (Tables 1 and 2), it is concluded that the formulations being used are correct. The results obtained from each of these three methods agree within statistics as predicted. For problem 2, there is a slight difference between results obtained from the Surface Integral Approximate method and the other methods, but this difference was expected due to the approximation itself.

Problem 3, as described in Fig. 2, is a three-dimensional problem, but it can be replaced by an equivalent one-dimensional problem by replacing the point source by an equivalent spherical shell source of radius R whose origin is at the center of the perturbing spherical shell. This equivalent one-dimensional problem is what was analysized to obtain the ANISN results of Table 3. All other results was a direct analysis of the problem as described in Fig. 2, i.e., the unperturbed flux was for the point source in an infinite air medium, and the adjoint flux was for the water - iron perturbing region as shown. The results at the different separation distances R for the Adjoint Difference and the Surface Integral Approximate methods were obtained for a single adjoint

TABLE 2

RESULTS FOR PROBLEM 2

Method	Histories	Fluence	Comments
ANISN		1.33×10^{-13}	
Adj. Diff.	4,000	1.27×10^{-13}	S_4
Surf. Int.	4,000	1.20×10^{-13}	ANISN Calc.
Surf. Int. Approx.	4,000	1.51×10^{-13}	
ANISN		1.64×10^{-13}	
Adj. Diff.	50,000	1.56×10^{-13}(0.062)	S_{16} ANISN
Surf. Int.	40,000	1.53×10^{-13}	Calc.
Surf. Int. Approx.	40,000	1.92×10^{-13}(0.033)	

*The numbers in the parenthesis are the fractional standard deviation of the reported results based on the Monte Carlo calculations.

TABLE 3

RESULTS FOR PROBLEM 3[a]

R (meters)	ANISN	Adj. Diff. (fsd) 10,000 histories	Surf. Int. Approx. (fsd) 10,000 histories	Adjoint Monte Carlo (fsd) 10,000 histories	Unperturbed ANISN[b]
200	1.209	1.223(0.075)	1.159(0.046)	1.142(0.10)	2.095
400	0.736	0.750	0.713	0.802(0.14)	1.338
600	0.340	0.341(0.059)	0.320(0.041)	0.345(0.16)	0.636
800	0.143	0.137	0.131	0.146(0.20)	0.260
1000	0.0542	0.0508(0.059)	0.0474(0.042)	0.0555(0.26)	0.0975

[a]All results in this table are the computed results multiplied by $4\pi R^2$. All ANISN calculations are S_{16}.

[b]This is the fast flux in the air with the perturbing medium removed.

Monte Carlo calculation for each method. The results for the Adjoint Monte Carlo method required a Monte Carlo calculation for each separation distance. From this problem it was concluded that the formulations used for breaking the overall problem up into two independent separate problems and followed by the combination of results to obtain the effect of interest are correct.

D. Problems 4, 5, and 6

The unperturbed problem consists of a unit point fission source in an infinite air medium. In each of these three (unlike the first three problems considered) problems, the effect of interest is dependent on the orientation of the perturbing medium (vehicle) relative to the source. Problems 4 and 5 consists of the same vehicle with different detectors. In the analysis which were carried out with Problems 4 and 5, it was found that a relatively large amount of computer time was required due to the use of the generalized geometry package in MORSE; therefore, Problem 6 was introduced which has the same general features of Problems 4 and 5 and does not require the more generalized geometry routines. Therefore, statistically more precise results were obtained for Problem 6.

Description of Problems 4, 5, and 6. In Problem 4, the perturbing medium was taken to be the vehicle, made of iron, shown in Fig. 3. The effect of interest was the fast flux for the point detector located as shown in Fig. 3. Problem 5 differs only from Problem 4 through the fast flux detector. In particular, Problem 5 consists of a six inch diameter spherical detector centered at the same point as the point detector of Problem 4.

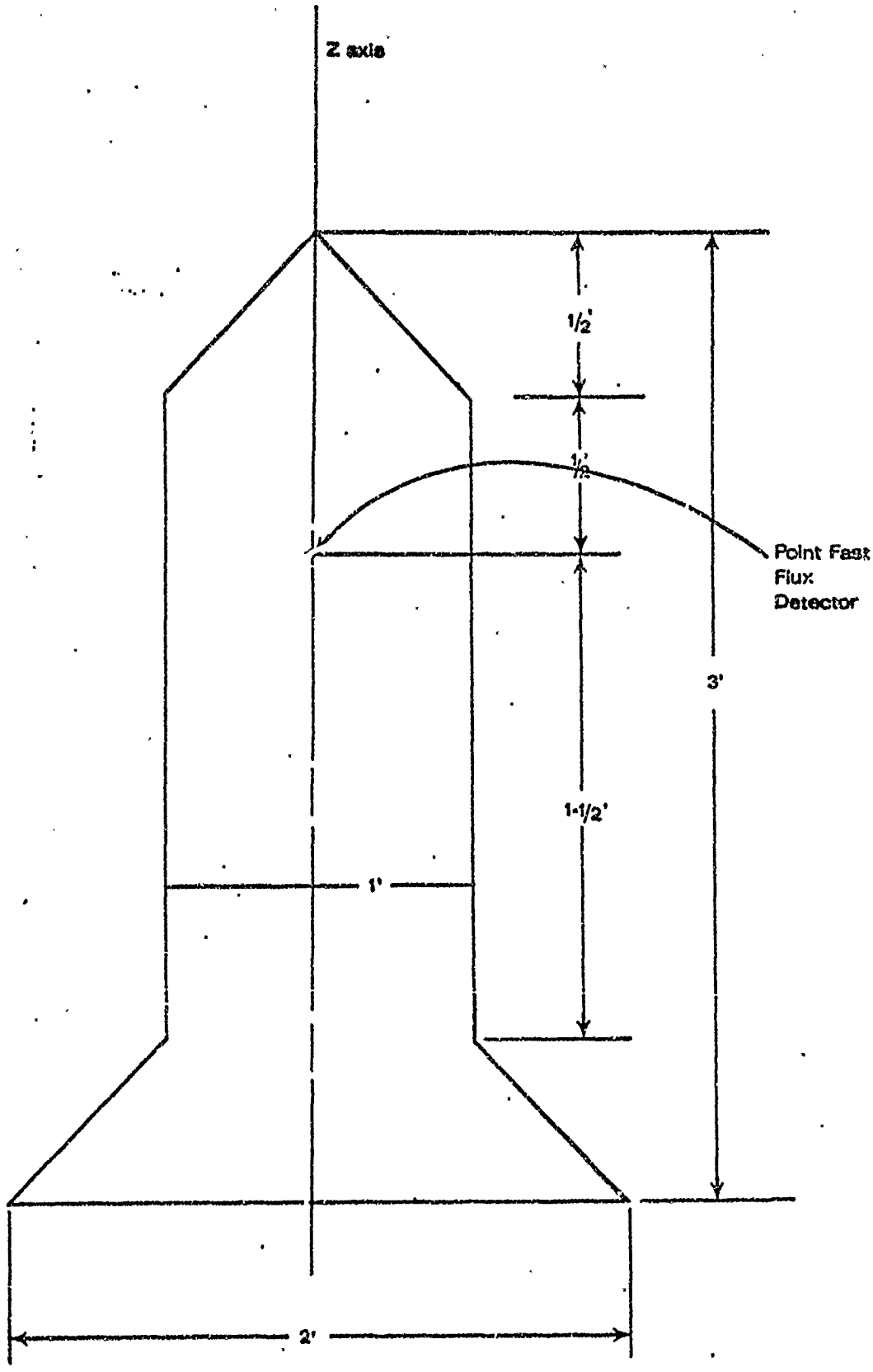

Figure 3. Geometric Configuration for Problem 4.

Three different orientations of the vehicle (called rocket from henceforth) are considered for Problems 4 and 5. These are:

1. The rocket is moving around the source at a distance R away such that the z-axis is perpendicular to a straight line connecting the source point and the detection point.
2. The nose of the rocket is moving away from the source.
3. The nose of the rocket is moving toward the source.

Problem 6 consists of the iron parallelpiped shown in Fig. 4.* The effect of interest is the same as in the previous problems (the fast flux). The fast flux is desired for three orientations of the parallelpiped at each specified distance between the source and the detector. These orientations are illustrated by the Roman numerals in Fig. 4. The numerals represent the source direction relative to the parallelpiped.

Results for Problems 4, 5, and 6. The computed fast flux for Problems 4 and 5 and presented in Tables 4 and 5 for each of the indicated rocket orientations. The fractional standard deviations in all of the results presented in Tables 4 and 5 are on the order of 25%.

The fast flux multiplied by $4\pi R^2$ (R is the distance in meters from the source to the detector) obtained for Problem 6 are presented in Table 6. The fractional standard deviation is less than 10% for all cases presented for Problem 6 as indicated in Table 6.

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*Problems 4 and 5 were found to consume a large amount of computer time due to the generalized geometry package; therefore, we choose the parallelpiped to continue the source-vehicle orientation study. This geometry requires relatively little computer time.

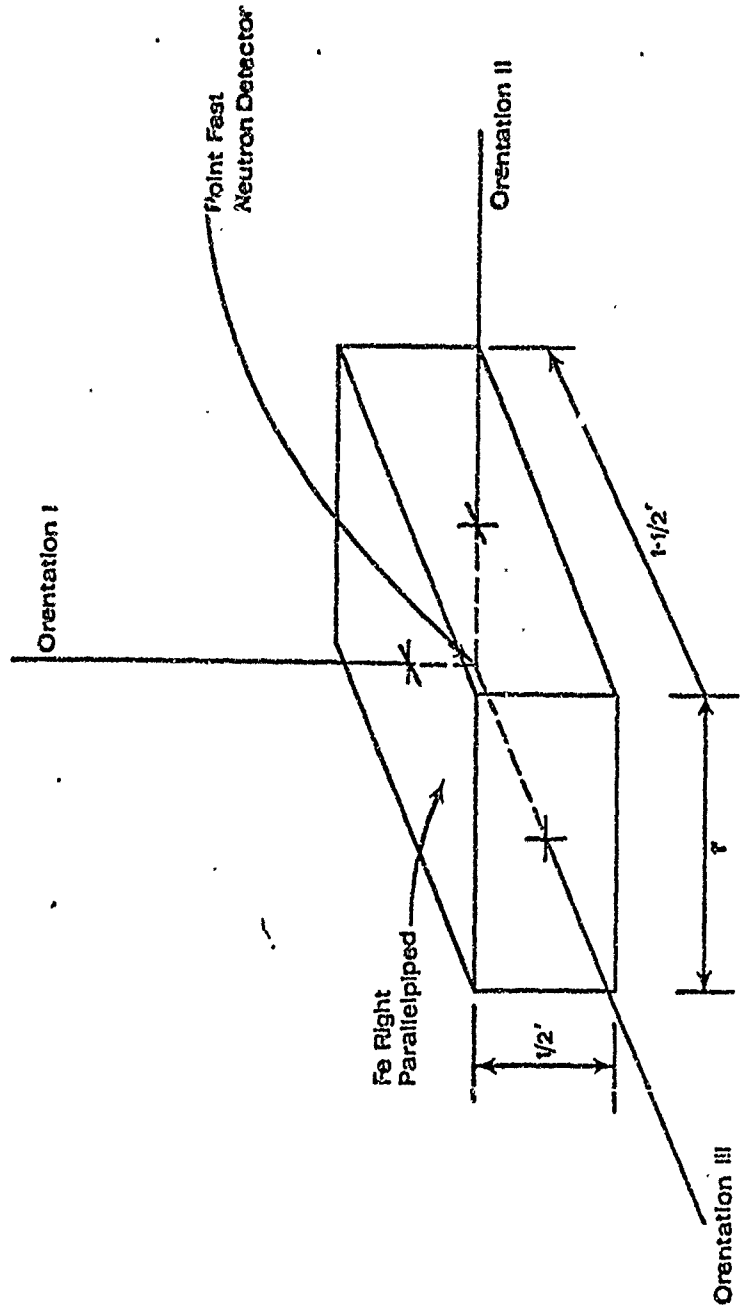

Figure 4: Geometric Configuration for Problem 6.

TABLE 4

RESULTS FOR PROBLEM 4[a]

Distance from Source Meters	Adj. Diff.	Surf. Int. Approx.
Around Source		
200	3.641×10^{-10}	3.474×10^{-10}
400	5.128×10^{-11}	5.565×10^{-11}
600	1.026×10^{-11}	1.100×10^{-11}
800	2.254×10^{-12}	2.399×10^{-12}
1000	5.035×10^{-13}	5.560×10^{-13}
Away From Source		
200m	2.937×10^{-10}	3.137×10^{-10}
400	4.430×10^{-11}	5.192×10^{-11}
600	9.067×10^{-12}	1.046×10^{-11}
800	2.014×10^{-12}	2.315×10^{-12}
1000	4.527×10^{-13}	5.421×10^{-13}
Toward Source		
200m	3.251×10^{-10}	4.389×10^{-10}
400	4.816×10^{-11}	6.508×10^{-11}
600	9.829×10^{-12}	1.296×10^{-11}
800	2.182×10^{-12}	2.829×10^{-12}
1000	4.904×10^{-13}	6.516×10^{-13}

[a]ANISN calculations were S_4. Estimates for Adjoint flux were based on 4,000 histories.

TABLE 5

RESULTS FOR PROBLEM 5[a]

Distance from Source Meters	Adj. Diff.	Surf. Int. Approx.
Around Source		
200	4.390×10^{-10}	3.448×10^{-10}
400	6.840×10^{-11}	5.568×10^{-11}
600	1.433×10^{-11}	1.172×10^{-11}
800	3.267×10^{-12}	2.689×10^{-12}
1000	7.830×10^{-13}	6.459×10^{-13}
Away From Source		
200m	3.513×10^{-10}	2.920×10^{-10}
400	6.124×10^{-11}	4.750×10^{-11}
600	1.329×10^{-11}	1.031×10^{-11}
800	3.078×10^{-12}	2.404×10^{-12}
1000	7.435×10^{-13}	5.830×10^{-13}
Toward Source		
200m	3.858×10^{-10}	3.976×10^{-10}
400	6.580×10^{-11}	6.463×10^{-11}
600	1.420×10^{-11}	1.351×10^{-11}
800	3.281×10^{-12}	3.071×10^{-12}
1000	7.916×10^{-13}	7.327×10^{-13}

[a]All results are based on 5,000 adjuncton histories and S_{16} angular fluxes. The tabulated values are spatially averaged fast flux fluences.

TABLE 6

RESULTS FOR PROBLEM 6
($4\pi R^2$ * Fast Flux)

R (Meters)	Adj. Diff.	Surf. Int. Approx.
Orientation I		
200	2.268 (0.051)[a]	2.268 (0.056)
400	1.336 (0.034)	1.369 (0.058)
600	0.619 (0.029)	0.636 (0.059
800	0.250 (0.027)	0.255 (0.059)
1000	0.0931(0.026)	0.0951(0.060)
Orientation II		
200	1.772 (0.075)	1.819 (0.058)
400	1.156 (0.046)	1.171 (0.058)
600	0.558 (0.038)	0. 61 (0.058)
800	0.229 (0.035)	0 228 (0.059)
1000	0.0864(0.033)	0.0857(0.059)
Orientation III		
200	1.563 (0.088)	1.590 (0.059)
400	1.078 (0.053)	1.077 (0.060)
600	0.525 (0.045)	0.524 (0.061)
800	0.216 (0.041)	0.214 (0.062)
1000	0.0815(0.039)	0.0810(0.063)

[a]Fractional standard deviations in parentheses.

The calculational procedure followed in Problems 4 and 5 differed from that pursued in Problem 6. In particular, the procedure used in Problems 4 and 5 was the three step procedure outlined in Sec. II of this report. The technique employed in Problem 6 was to evaluate Eq. 7 (for the Surface Integral Approximation) or Eq. 11 (for the Adjoint Difference) directly in the Monte Carlo code MORSE.

Discussion of Results for Problems 4, 5, and 6. From the results obtained for Problems 4 and 5, it is concluded that the three-step procedure outlined earlier in this report is valid. In particular, we can obtain the effect of interest within the target for different source-target orientations by using a single forward flux calculation for the source in air problem and a single adjoint flux calculation for the target in air problem. However, it was also found for a generalized application of this three-step technique, further development is required to properly interface the results obtained from the two independent calculations. The problems are introduced by (a) the use of different reference coordinate systems in the two calculations and (b) coupling the results obtained from deterministic calculational techniques.

The results for Problem 6 were obtained by (a) evaluate the "response function" using the forward flux and the coordinate system used in the forward flux calculation, (b) transform the response function to the coordinate system to be used in the adjoint (Monte Carlo) flux calculations, and (c) evaluate the effect of interest directly in the Monte Carlo code using the transformed response function. The disadvantage with this procedure is that an adjoint calculation is required for each

target-vehicle orientation.* This approach was adopted to (a) circumvent the problems encountered in the Problems 4 and 5, and (b) to establish a reference calculational technique for the more generalized techniques which are to be developed to utilize the three step calculational techniques.

E. Problem 7

Description. The unperturbed problem is that of calculating the angular fluxes due to a unit point fission source located 50 feet above an air-ground interface. This is a two-dimensional (r-z cylindrical geometry) problem. This problem was solved by E. A. Straker[5] with the discrete ordinates code DOT. The unperturbed fluxes used in this problem were taken from Straker's work.

The perturbation to this system is a two-foot right concrete cylinder. At the center of this cylinder is a three inch cubic detector. The detector measures the average fast fluence (E>.1 Mev) in the detector volume. The geometric configuration is illustrated in Figure 5. The concrete (with rebar) and ground (8.5 weight percent water) compositions are shown in Table 7.

Scoring Surface for the Conventional Method. In previous problems, the surface used in the conventional method was the surface of the

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*This technique is still preferable over the more direct approach of explicitly accounting for the source and target in a single calculation. The difficulty with the single calculation is the normally large separation between the target and source which is a deep penetration geometrically complex problem.

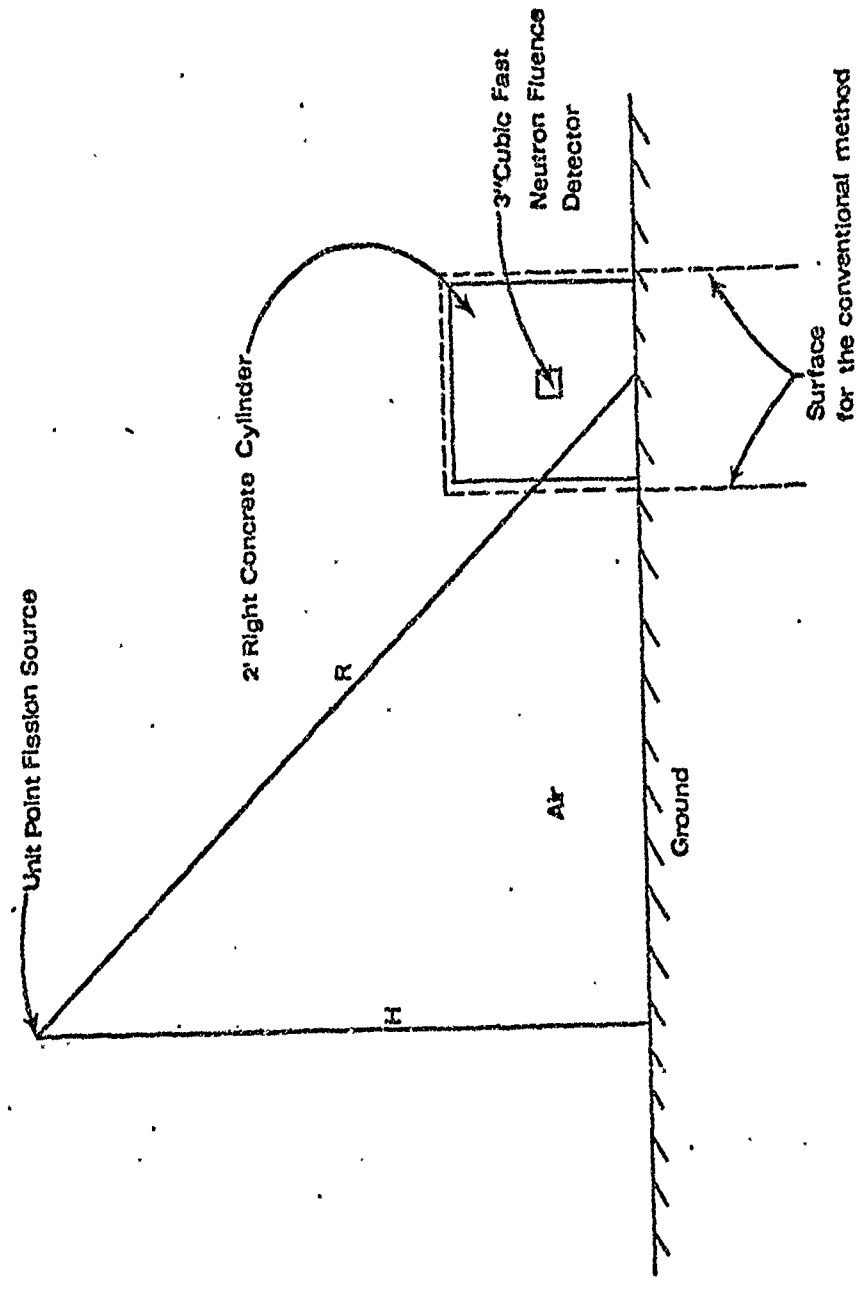


Figure 5: Geometric Configuration for Problem 7.

TABLE 7

MATERIAL COMPOSITIONS

(Number Density x 10^{-24})

Element	Concrete & Rebar ($2.62\ gm/cm^3$)	Ground ($1.6\ gm/cm^3$)
O	4.084 E-2	3.036 E-2
Si	1.332 E-2	9.990 E-3
Al	2.738 E-3	2.040 E-3
Fe	5.269 E-3	2.400 E-4
Mg	1.620 E-4	1.200 E-4
Ca	2.426 E-3	1.800 E-3
Na	1.071 E-3	8.000 E-4
K	8.280 E-4	6.200 E-4
H	1.065 E-2	7.600 E-3
Ti	2.600 E-5	2.000 E-5
Mn	7.500 E-5	2.000 E-5
S	8.400 E-5	6.000 E-5
C	1.310 E-4	- - - -
P	5.000 E-6	- - - -
Ni	1.300 E-4	- - - -
Cr	1.200 E-5	- - - -
Mo	1.800 E-5	- - - -
Cu	1.500 E-5	- - - -

perturbing material. In this problem, however, the inward directed perturbed flux will be considerably less than the inward directed unperturbed flux at the surface of the cylinder in contact with the air-ground interface. Therefore, the surface sketched in Figure 4, which extends in the vertical direction to minus infinity, was used.

The forward and adjoint fluxes decrease rapidly with distance below the air-ground interface. (The mean free path in ground is about two centimeters.) Therefore, the contribution to the effect of interest in the conventional method of the surface below the interface was assumed insignificant.

Results for Problem 2. The unperturbed, DOT, calculations were S_8 (40 discrete directions). The cross sections used in DOT and MORSE were 22 group, P_3. The adjoint Monte Carlo calculations involved following 20,000 histories. Since the perturbation greatly reduced the fast fluence, the change in the effect of interest is reported in Table 8, i.e., for the adjoint difference,

$$\Delta\lambda = \int \psi^*(\bar{p})\ f(\bar{p})d\bar{p}. \tag{14}$$

and for the conventional,

$$\Delta\lambda = \int_{\text{Det}} R(\bar{p})\ \phi_2(\bar{p})d\bar{p} + \int_{\text{Surface}} (\bar{\Omega} \cdot n)_{in}\ \phi_2(\bar{p})\ \phi^*(\bar{p})d\bar{p}. \tag{15}$$

Discussion of Results for Problem 7. In Table 8, the obvious difference between the surface integral approximation and the adjoint difference method is the statistical uncertainty. In particular, the fractional standard deviations for the surface integral approximation are observed to be very low. This effect can be accounted for by noting that Eq. (15) consists of adding a term calculated by Monte Carlo

techniques to a term calculated by discrete ordinates techniques. For large perturbations, as was the case for this problem, the term calculated by Monte Carlo is small. Therefore, even a relatively large fractional standard deviation was in the Monte Carlo calculation will appear small overall. This effect is not observed in the adjoint difference method because the statistical uncertainty of the quantity calculated with Eq. (14) is a measure of the reproducibility of the Monte Carlo calculation alone.

The results from the two calculational techniques (surface integral and adjoint difference) agree with each other well. This was expected since little doubt exists as to how to choose the surface for the surface integral technique, but for some problems of this type, (a vehicle located at an air-ground interface for example) it may be difficult to choose the surface apriori. In such a situation, the adjoint difference technique would be preferable over the surface integral technique.

TABLE 8

RESULTS FOR PROBLEM 7[a]

R (Meters)	Adjoint Difference Method	Conventional Method
300	0.893 (0.078)[b]	0.882 (0.008)
600	0.249 (0.065)	0.253 (0.008)
900	0.0603 (0.061)	0.0620 (0.008)
1200	0.0135 (0.057)	0.0139 (0.008)
1500	0.00315(0.056)	0.00325(0.008)

[a]All results are ($4\pi R^2$ * change in fast fluence).

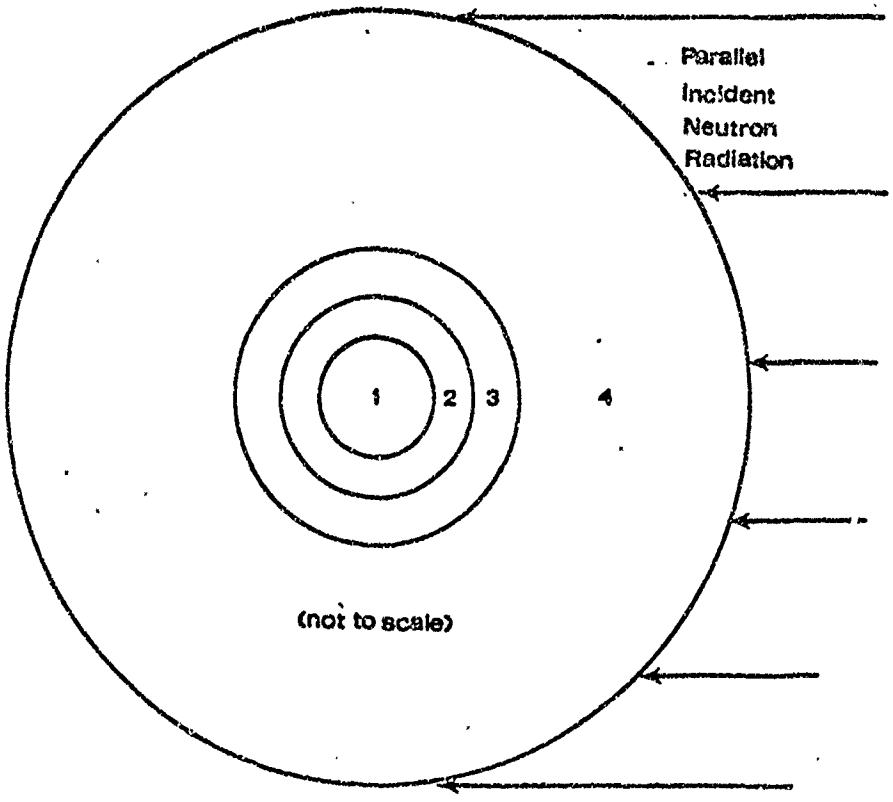
[b]Fractional standard deviation in parentheses.

IV. RESULTS FOR FISSILE PROBLEMS

The results for a single fissile problem are included in this report. The objective is to demonstrate the applicability of the adjoint mode of the MORSE code to problems of the type of interest which contain fissile material. The problem chosen is the "Calculation No. 2" problem presented in Ref. 6. The results will be compared with ANISN, and the ANTE-2 and DTF results presented in Ref. 6.

The problem is to compute the number of fissions per kilogram of U^{235} in the target shown in Fig. 6. The spherical target was subjected to a parallel incident neutron beam as shown. The incident neutron beam energy range from 14 Mev to thermal was broken up into a 25 group structure as given in Table 9. The fission cross section given in Table 9 was used as the response function. The results are presented in Fig. 7 as a function of the incident neutron energy over the energy range covered from group 1 through group 18.

The discrepancies between the ANTE-2 and DTF results were attributed to the different cross sections used.[5] The same cross section set was used in MORSE and ANISN (but different than those used in Ref. 6). Therefore, we conclude that the agreement between all focus calculational tools are as good as can be expected. From these results, it is concluded that the adjoint mode of MORSE can be applied to problems containing fissile materials. The calculational procedure employed in this sample problem was basically the surface integral approximation;



Region	Material	Inner Radius (cm)	Outer Radius (cm)	Material Density (atoms/cm^{3}x10^{-24})
1	VOID	0.0	0.8	.....
2	U-235	0.8	1.0	.04806
3	BN(B-19.7%B^{10})	1.0	1.2	.1364
4	CH_2	1.2	6.2	.1170

Figure 6. Configuration for a Fissile Sample Problem.

TABLE 9

ENERGY BAND STRUCTURE FOR FISSILE SAMPLE PROBLEM

Group	Energy		$\sigma_f(U^{235})$
1	12 - 14.	Mev	1.92967
2	8.3 - 12		1.79722
3	5.3 - 8.3		1.36285
4	3.4 - 5.3		1.25280
5	2.2 - 3.4		1.30383
6	1.4 - 2.2		1.24789
7	0.9 - 1.4		1.18587
8	.58 - 0.9		1.15389
9	370 - 580	kev	1.17654
10	240 - 370		1.26027
11	150 - 240		1.39574
12	100 - 150		1.57489
13	31 - 100		2.25959
14	10 - 31		3.15976
15	3.16 - 10		4.20512
16	1.0 - 3.16		6.37329
17	.316 - 1.0		11.4185
18	100 - 316	ev	20.3925
19	31.6 - 100		33.9860
20	10 - 31.6		57.2095
21	3.16 - 10		38.5393
22	1.0 - 3.16		28.3100
23	.316 - 1.0		84.6518
24	.076 - .316		241.256
25	.015 - .026		577.347

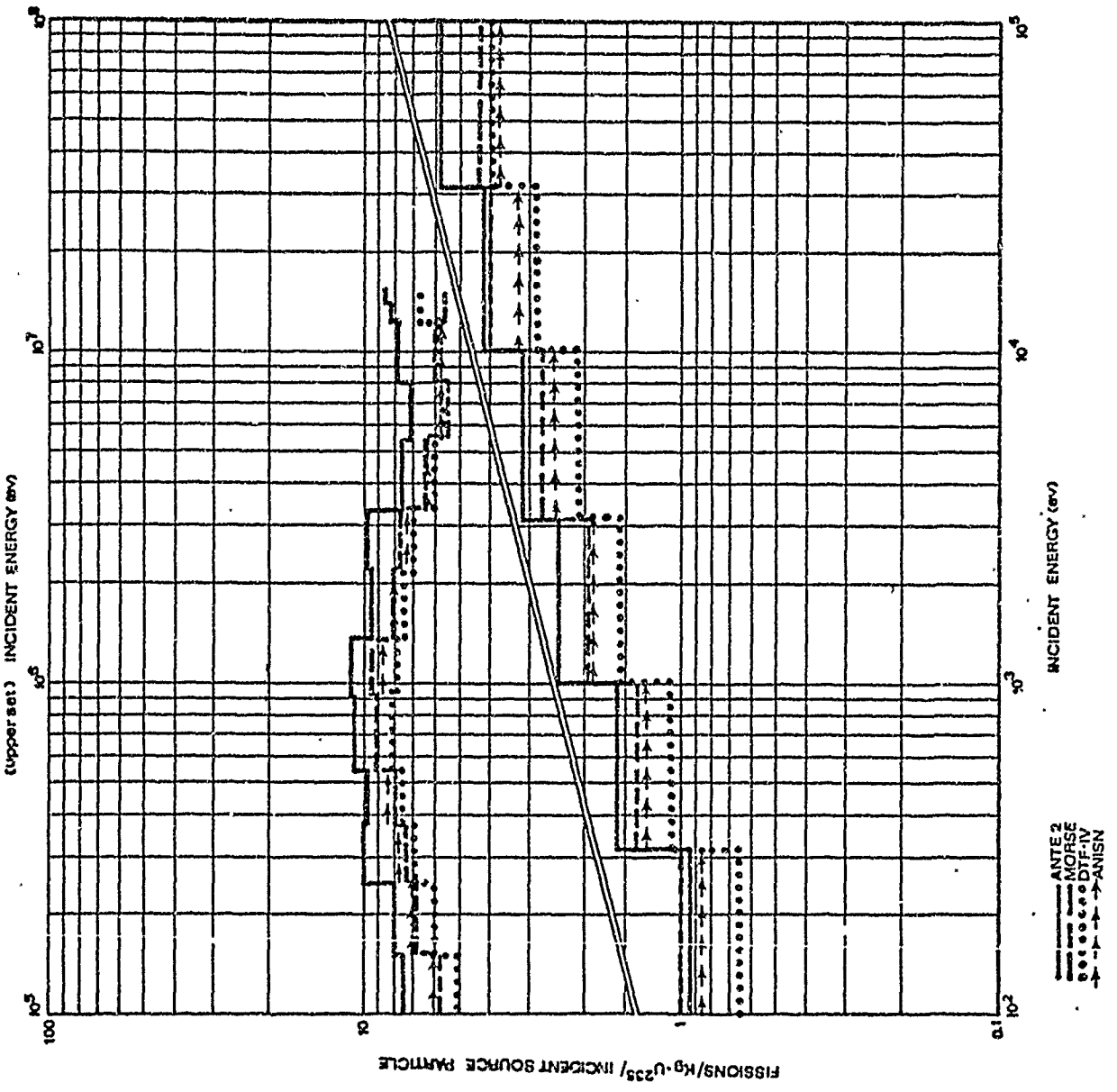


Figure 7. Fissile Sample Problem Comparison.

therefore, we have established that the techniques applied to the non-fissile problems can be extended to fissile problems. The specific problems encountered will be reported at a later date along with specific examples.

V. SUMMARY

In this report, a brief theoretical development was presented for the adjoint difference and surface integral techniques for solving a certain class of deep penetration geometrically complex radiation transport problem. The reader was referred to Ref. 4 for a more thorough theoretical development. In Ref. 4, a selected amount of calculated results for targets were presented to demonstrate the accuracy of the theoretical developments. In this report, all results obtained in this study for targets which do not contain fissile materials are presented. Furthermore, some preliminary results are presented for a target which does contain fissile materials are presented and compared with results reported in the literature.

From the overall results presented in this report, it is obvious that the adjoint difference and surface integral methods both lead to acceptable results. In general, it appears (based on results from the non-fissile problems) that the adjoint difference method is advantageous for those problems in which the target introduces a small perturbation and the surface integral approximation is advantageous (provided an adequate "scoring" surface can be identified apriori) for those problems in which the target introduces a large perturbation. These conclusions cannot be carried over to problems containing fissile materials at this time (they will be explored via examples and reported at a later date).

At this time, the utility of the three steps presented in the introduction has not been fully realized due to the complexity of Step 3 for

a target. This phase of the overall problem will be explored further and reported at a later date.

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