THE SEARCHLIGHT PROBLEM
FOR NEUTRONS IN A SEMI-INFINITE MEDIUM

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ABSTRACT

The solution of the Search Light Problem for monoenergetic neutrons in a semi-infinite medium with isotropic scattering illuminated at the free surface is obtained by several methods at various planes within the medium. The sources considered are a normally-incident pencil beam and an isotropic point source. The analytic solution is effected by a recently developed numerical inversion technique applied to the Fourier-Bessel transform. This transform inversion results from the solution method of Rybicki, where the two-dimensional problem is solved by casting it as a variant of a one-dimensional problem. The numerical inversion process results in a highly accurate solution. Comparisons of the analytic solution with results from Monte Carlo (MCNP) and discrete ordinates transport (DORT) codes show excellent agreement. These comparisons, which are free of any associated data or cross section set dependencies, provide significant evidence of the proper operation of both the transport codes tested.

I. INTRODUCTION

The use of personal computers (PCs) and workstations for complex scientific computation has expanded rapidly during the past few years. This trend is anticipated to continue in the future with the introduction of increasingly sophisticated microprocessors and microcomputer systems. For a number of reasons including security, economy, user convenience and productivity, an integrated system of neutronics and radiation transport software suitable for operation in the PC computational environment has been under development at the Idaho National Engineering Laboratory (INEL) over the past four years. Comprehensive computations that were only possible on a mainframe a few years ago can now routinely be performed on a PC using this software. At present, the system includes modules for processing of basic Evaluated Nuclear Data File (ENDF/B) data into application specific cross section sets, and for various types of neutron transport and diffusion theory calculations. Modules for one- and two-dimensional discrete ordinates transport, three-dimensional Monte Carlo, and for one-, two- and three-dimensional finite-difference diffusion theory analyses are currently available.

In order to provide the necessary verification of the PC software, the development of a complimentary analytical benchmark library has also been initiated. The major purpose of this library is to provide confidence that the PC codes, or any comparable codes for that matter, are properly coded and are operating properly. At present, only zero- and one-dimensional analytical benchmarks have been established in connection with this effort. In this presentation, a two-dimensional transport benchmark called the searchlight problem (SLP) will be presented. The SLP was first successfully evaluated using the F_n method which

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did not take advantage of the analytical features of the solution for the special cases considered here. This presentation will consider a simplified version of the SLP in a half-space having analytical solutions for the scalar flux at the free surface which have never been numerically evaluated.

In several papers recently appearing in the literature¹⁻³, the classical two-dimensional searchlight problem originally proposed by Chandrasekhar⁴ in the radiative transfer context was considered from the numerical point of view. Previously, the searchlight problem was shown to be expressible as a variant of a one-dimensional problem^{5,6} which provided an analytical solution that could, in principle, be numerically evaluated. The focus of this work is on the solution of the searchlight problem for monoenergetic neutrons in an isotropically scattering semi-infinite medium illuminated at the free surface. The solution is found using a new numerical evaluation and comparisons to well established codes are presented.

II. THEORY

The appropriate monoenergetic neutron transport equation in cylindrical geometry can be written as⁵

$$\left[\mu \frac{\partial}{\partial z} + \vec{\omega} \cdot \frac{\partial}{\partial \vec{\rho}} + 1 \right] \Phi(z, \vec{\rho}, \vec{\Omega}) = \frac{c}{4\pi} \int_{4\pi} d\vec{\Omega}' \Phi(z, \vec{\rho}, \vec{\Omega}'), \quad (1a)$$

and the boundary conditions for a beam are

$$\Phi(0, \vec{\rho}, \vec{\Omega}) = S(\vec{\rho}) \delta(\mu - \mu_0) \delta(\phi - \phi_0), \quad \mu > 0 \quad (1b)$$

and

$$\lim_{z \rightarrow \infty} \Phi(z, \vec{\rho}, \vec{\Omega}) < \infty. \quad (1c)$$

The desired quantity will be the scalar flux

$$\Phi(z, \vec{\rho}) = \int_{4\pi} d\vec{\Omega} \Phi(z, \vec{\rho}, \vec{\Omega}). \quad (2)$$

II.1 The transformed equation

When the multidimensional Fourier transform is applied to Eqs. (1), we obtain the following transformed equation

$$\left[\mu \frac{\partial}{\partial z} + u(\vec{\Omega}, \vec{k}) \right] \bar{\Psi}(z, \vec{\Omega}; \vec{k}) = \frac{c}{4\pi} \int_{4\pi} d\vec{\Omega}' \bar{\Psi}(z, \vec{\Omega}'; \vec{k}) \quad (3a)$$

with

$$u(\vec{\Omega}, \vec{k}) \equiv 1 - ik(1 - \mu^2)^{1/2} \cos(\phi - \psi)$$

and

$$\bar{\Psi}(0, \vec{\Omega}; \vec{k}) = \bar{S}(\vec{k}) \delta(\mu - \mu_0) \delta(\phi - \phi_0), \quad \mu > 0 \quad (3b)$$

$$\lim_{z \rightarrow \infty} \bar{\Psi}(z, \vec{\Omega}; \vec{k}) < \infty. \quad (3c)$$

The transformed quantities are defined as

$$\bar{\Psi}(z, \bar{\Omega}; \bar{k}) = \int d\bar{\rho} e^{i\bar{k} \cdot \bar{\rho}} \Psi(z, \bar{\Omega}, \bar{\rho}) \quad (4a)$$

$$\bar{S}(\bar{k}) = \int d\bar{\rho} e^{i\bar{k} \cdot \bar{\rho}} S(\bar{\rho}). \quad (4b)$$

From the Fourier inversion theorem, the scalar flux is therefore

$$\Phi(z, \bar{\rho}) = \frac{1}{(2\pi)^2} \int d\bar{k} e^{-i\bar{k} \cdot \bar{\rho}} \bar{\Psi}(z; \bar{k}) \quad (5a)$$

where the transformed scalar flux is

$$\bar{\Psi}(z; \bar{k}) = \int_{4\pi} d\bar{\Omega} \bar{\Psi}(z, \bar{\Omega}; \bar{k}). \quad (5b)$$

II.2 Integral equation for $\bar{\Psi}(z; \bar{k})$

Eqs. (3) can be recast as an integral equation for the scalar flux by reformulation of the integro-differential equation along the characteristics of particle motion which, when integrated over direction, gives (the k dependence has been suppressed)

$$\Psi(z) = F(z) + \frac{c}{2} \int_0^\infty dz' K(|z - z'|) \Psi(z'). \quad (6a)$$

After some manipulation, the kernel becomes³

$$K(z) = \int_0^1 \frac{d\mu}{\mu} \frac{e^{-z(1+(k\mu)^2)^{1/2}/\mu}}{(1+(k\mu)^2)^{1/2}}, \quad (6b)$$

with

$$F(z) = e^{-z/U_0} \bar{S}(\bar{k}). \quad (6c)$$

With this form of the kernel, an equivalent pseudo-problem can be identified which allows for the determination of Ψ .

II.3 The pseudo-problem

Consider the following generalized transport equation:

$$\left[\mu a(\mu) \frac{\partial}{\partial z} + b(\mu) \right] \phi(z, \mu; \mu^*) = \frac{c}{2} \int_{-1}^1 d\mu' \phi(z, \mu'; \mu^*) \quad (7a)$$

$$\phi(0, \mu; \mu^*) = Q_0 \delta(\mu - \mu^*); \quad \mu^*, \mu > 0 \quad (7b)$$

$$\lim_{z \rightarrow \infty} \phi(z, \mu; \mu^*) < \infty. \quad (7c)$$

In addition, a and b are required to be non-negative, even functions of μ . Again applying integral transport theory to Eqs. (7) yields the following integral equation:

$$\phi(z; \mu^*) = e^{-z/\xi^*} + \frac{c}{2} \int_0^\infty dz' K(|z - z'|) \phi(z'; \mu^*), \quad (8)$$

where

$$K(z) = \int_0^1 \frac{d\mu}{\mu} e^{-zb(\mu)/(a(\mu))}. \quad (9)$$

For specific functions a and b , the following equivalence can be shown to hold:

$$\bar{\Psi}(z) = \bar{\phi}(z). \quad (10)$$

The solution to Eq. (8) is obtained by following the method of Chandrasekhar⁴ yielding

$$\phi(0, -\mu; \mu^*) = \frac{c}{2} \frac{1}{\mu a(\mu)} \frac{\xi \xi^*}{\xi + \xi^*} H(\xi^*; k) H(\xi; k), \quad (11)$$

where the H -function satisfies the following non-linear integral equation:

$$H(\xi; k) = 1 + \frac{c}{2} \xi H(\xi; k) \int_0^1 \frac{d\mu'}{b(\mu')} \frac{H(\xi'; k)}{\xi + \xi'}, \quad (12)$$

and

$$\phi(0; \mu^*) = H(\xi^*; k). \quad (13)$$

Therefore, from Eq. (10), the transformed flux at $z = 0$ is

$$\bar{\Psi}(0; \vec{k}) = \bar{S}(\vec{k}) H(U_0; k). \quad (14)$$

The interior flux is obtained using the integral transport equation evaluated at $z = 0$ to give

$$\bar{\Psi}(z; \vec{k}) = \bar{S}(\vec{k}) U_0 H(U_0; k) \mathcal{L}_z^{-1} \left[\frac{H(\frac{1}{s}; k)}{1 + s U_0} \right]. \quad (15)$$

II.4 The Fourier Inversion

The inversion formula for normally or isotropic incident fluxes is therefore

$$\Phi(z, \vec{\rho}) = \Phi(z, \rho) = \frac{1}{2\pi} \int_0^\infty dk k \bar{\Psi}(z; k) J_0(\rho k) \quad (16)$$

where $J_0(u)$ is the Bessel function of zeroth order. Thus the scalar flux will depend only on ρ and z , and not on azimuth.

From Eq. (14), and for a normally incident beam ($\mu_0 = 1$ implying $U_0 = 1$), we have for the exiting flux

$$\phi(0, \rho) = \frac{1}{2\pi} \int_0^\infty dk k \bar{S}(k) H(1; k) J_0(\rho k) \quad (17a)$$

and, for $z > 0$ by identifying the exiting fluxes with the Laplace transform of the interior flux, we have

$$\Phi(z, \rho) = \frac{1}{2\pi} \int_0^\infty dk k H(1; k) \mathcal{L}_z^{-1} \left[\frac{H(\frac{1}{s}; k)}{1+s} \right] \quad (17b)$$

with corresponding inversions for the isotropically impinging and uniformly distributed sources.

III. NUMERICAL IMPLEMENTATION OF THE ANALYTICAL SOLUTION

The evaluation of the scalar flux in the interior and at $z = 0$ presents a significant numerical challenge. In particular, the Fourier-Bessel transform inversion must be performed on a rather complicated image function, which itself will contain additional integrations and possibly a Laplace transform inversion. The three major numerical procedures required are the evaluation of the H-function, the numerical Fourier-Bessel inversion, and the numerical Laplace transform inversion. The latter algorithm is found in Ref. 8, and will not be discussed here.

The evaluation of the H-function is central to the numerical determination of the scalar flux and current density. The defining integral equation to be solved for the H-function can be rearranged by a change of variable in order to avoid an almost singular point at large k . In effect, the singular portion of the integrand is eliminated, allowing the use of a standard shifted Legendre-Gauss quadrature. A two step iterative algorithm is used to evaluate the H-function to a high degree of accuracy.

The second numerical procedure involves the Fourier-Bessel inversion of the form

$$I = \frac{1}{2\pi} \int_0^\infty du u f(u) J_0(\rho u). \quad (18)$$

The most straightforward evaluation of I is to break up the integration over the intervals between the zeros of J_0 , resulting in an infinite series. The series convergence is then accelerated using the Euler-Knopp transformation or epsilon algorithm.

In a performance study and the comparisons to follow, several radial source configurations were considered, including point and disk sources. It should be noted that, in principle, any source with a Fourier transform can be accommodated.

Before providing comparisons between the analytical benchmarks and well established transport codes, it was crucial to first set the parameters governing the numerical algorithm for the benchmark. The major parameters are the quadrature order for the evaluation of the H-function, and the error associated with the truncation of the series required in the evaluation of both the Fourier and Laplace inversions⁸. In addition, there are internal checks for both inversions in order to detect a loss of significance. If so, the convergence criterion for the evaluation of the integrals contained in each term of the series representing the inversion was reduced accordingly until the desired significance was achieved.

IV. COMPARISONS WITH TRANSPORT CODE RESULTS

IV.1 Comparison with Stochastic Transport Results

The solution of the SLP was also computed using the MCNP⁹ continuous energy three-dimensional coupled neutron-photon Monte Carlo code. This presented a challenging problem, as it is generally unwise to explicitly model infinite media in a stochastic code, and also because the necessary idealized one-group cross sections did not exist. Additionally, because the internal surface solutions required penetrations of many (>10) mean free paths, deep penetration statistical concerns were involved, entailing tracking a great number of particle histories. Variance reduction techniques, although available in the MCNP code, were not employed. This reduced the problem to a pure test of the MCNP code algorithms.

To alleviate some of these barriers, the semi-infinite medium was modelled as a large (100 mfp) radius hemisphere, with free surfaces at the interface and outer spherical boundaries. The source neutrons are incident at the free surface, with the source centered at the origin. This simulated the semi-infinite medium accurately, but did not allow particles to be tracked indefinitely. This approximation introduced some error into the solution. An evaluation of the error incurred in using a finite medium was performed by computing the surface integral of the current exiting the medium. As expected, this integral was identically zero, as the error is bounded above by e^{-160} , which is the maximum probability that a neutron will be transported from the last tally position to the outer boundary and then return to the tally position.

A one-group cross section set was constructed for two fictitious isotopes: one purely absorbing, the other purely scattering with an infinite ($A = 300$) mass to remove the differences between the CM and lab coordinate systems. This allowed a wide range of idealized configurations to be modelled easily. Flux values were evaluated at the free surface of the semi-infinite medium, and at several internal surfaces normal and parallel to the free surface. Solutions for surfaces at penetration depths of up to 10 mean free paths were evaluated.

Several cases were modelled for the flux at the free surface for both the 0.99 scattering, 0.01 absorbing and 0.8 scattering, 0.2 absorbing media. Point and disk sources, for both beam and isotropic angular distributions, were used for both media. For the internal surfaces ($z > 0$), only the point beam source in the 0.99 scattering medium was considered. In each case, the total cross section was set to 1cm^{-1} .

Calculated results for the scalar flux at the free and internal surfaces for various radii between 0 and 10cm are shown in Figures 1 - 6. Agreement between the benchmark analytical solution and the MCNP results is excellent. The small deviations observed are due to the statistical nature of the Monte Carlo results, and are within 3σ of the benchmark solution. For the data at small radii, the fluctuations are mainly due to the small tally areas involved, while the large radius deviations are due mainly to particle attenuation effects. For all cases, the tally relative statistical errors are less than 5%, and less than 0.5% for the bulk of the data.

All MCNP cases were run on a DECstation 5000/200 workstation using MCNP version 4.2, and required between 15 and 5000 cpu minutes to complete cases involving 250,000 particle histories for the free surface cases and up to 32 million particle histories for the deep penetration internal surface solutions. These results, while not providing a full-scale verification of the code, show the proper operation of the MCNP code in a UNIX-based short word workstation environment.

IV.2 Comparison with Discrete Transport Results

Calculation of the searchlight problem using the DORT¹⁰ discrete ordinates method is also somewhat challenging because of the potential for ray effects and negative fluxes when computationally practical quadrature sets and mesh structures are used. In this work, the problem was modelled assuming one energy group,

isotropic scattering, and a cylindrical medium having an outside radius and height equal to 20 mfp. The total cross section was set to 1.0cm^{-1} . Calculations were performed for impinging beam radii of 0.5cm (to approximate the delta function beam) and 3cm. The beam was assumed to be monodirectional and perpendicularly incident at the center of the free surface in all cases. The scalar-weighted spatial differencing scheme and a symmetric S_{16} quadrature set (160 directions) were employed. Mesh intervals were 0.5cm in both the radial and axial directions for ρ and z between 0 and 10cm. From 10 to 20cm, the mesh intervals were set to 1cm in both dimensions.

Calculated results for the scalar flux at the free surface as a function of radius for radii between 0 and 10cm are shown for both beam sources and the isotropic source in Figures 1-4. (Beyond a radius of 10cm, one begins to see undesired boundary condition effects in the DORT results.) The data in Fig. 1 are for the case where the scatter cross section is set to 0.99cm^{-1} , relative to a total cross section of 1.0cm^{-1} . Agreement between the benchmark solutions and the discrete ordinates results is excellent for all sources. As expected, slight ray effects are seen in the DORT results for the small beam. The execution time for the DORT calculation was about 23 minutes on an IBM PS/2 Model 70 (16 MHz) running under DOS 4.0 with 640k addressable random access memory. Similar results were seen for the interior surface solutions, which are shown in Figures 5 and 6.

Calculated results were also obtained for isotropic incident sources and for the case where the scatter cross section was set to 0.8cm^{-1} . Similarly excellent agreement between the benchmark and the discrete ordinates results was observed. Although it does not constitute a complete, in-depth, code verification, this exercise has provided significant evidence of the proper operation of the DORT code module as adapted for operation in a 32-bit PC-based environment.

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Figure 1. Scalar flux at the surface of the searchlight problem geometry for two different impinging beam source radii. The total source strength is 1.0 in both cases.

Figure 2. Scalar flux at the surface of the searchlight problem geometry for two different impinging beam source radii. The total source strength is 1.0 in both cases.

Figure 3. Scalar flux at the surface of the searchlight problem geometry for two different impinging isotropic source radii. The total source strength is 1.0 in both cases.

Figure 4. Scalar flux at the surface of the searchlight problem geometry for two different impinging isotropic source radii. The total source strength is 1.0 in both cases.

Figure 5. Calculated fluxes along the z-axis at various radii for the Searchlight Benchmark.

Figure 6. Calculated fluxes along the r -axis at various axial positions for the Searchlight Benchmark. **DISCLAIMER**

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