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Neutron Diffusion Solutions for Homeland Security Applications

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ABSTRACT

As computing technology advances, better techniques become available for particle transport simulation. This project is aimed at developing a deterministic algorithm based on diffusion theory for neutron transport applications. The linear algebra method employed for solving the transport equations is finite-differencing. This project has resulted in a 3-D single energy, serial computer program called **S**erial **E**nvironment **N**eutral particle **DIFF**usion (SENDIFF), which can solve both fixed source and eigenvalue (criticality) problems. One potential use of SENDIFF is modeling radiation detection systems. To examine the capability of SENDIFF, a model was developed for a package containing weapons grade plutonium. A flux distribution was predicted by SENDIFF to identify the detection methodology necessary for the identification of the weapons grade plutonium. This paper demonstrates that SENDIFF can be used as a scoping tool for obtaining an approximate solution that includes sufficient information for identification of weapons grade plutonium. This is important because the more accurate approach of transport theory may require significant computation time. A transport calculation can necessitate large amounts of inspection time which may not be practical in some situations.

INTRODUCTION

In nuclear engineering, neutron flux is an important quantity to determine. Flux is a measure of the amount of neutrons passing through an area per unit time. Knowing the flux of neutrons is critical when determining how neutrons will interact with their surroundings. To detect nuclear materials, such as plutonium, it is essential to determine the flux of neutrons that is emitted. If models can be developed to describe how neutrons will flow through a medium, then detection methods can be refined and weapons material can be detected.

One of the most common theories used to determine neutron flux is diffusion theory. Diffusion theory is a simplification of the more complex transport theory. The major difference between the two theories is the fact that diffusion is valid only if the angular flux is linearly dependants on angle. This approximation enables us to use the Fick's law which provides a formulation for diffusion of neutrons from areas of high neutron density to areas of low neutron density. Diffusion theory is not accurate in media in which the neutron flux is highly angular dependant. Examples of this include near a boundary, in a strong absorbing material, or in a low density material.[1]

The primary benefit of this simplification is the computational savings. Diffusion problems are much simpler and quicker to solve than transport theory problems. However, if appropriate interaction cross-sections and diffusion coefficients can be generated, the solutions can also provide accurate results for most applications.

The computer code developed for this project was SENDIFF for **S**erial **E**nvironment **N**eutral particle **DIFF**usion. In this article, SENDIFF was used to investigate what detection methods would be the most accurate for homeland security applications. The model used was a 4.28 kg cube of plutonium packaged inside a cardboard box. This cardboard box was placed inside an iron shipping container. An assessment was made if a Helium-3 (He-3) detector (a sensitive neutron detector) would be able to detect the neutrons emitted from the plutonium.

FORMULATIONS

The following formulations are used to create a finite-difference solution to the Neutron Diffusion Equation.
The Neutron Diffusion Equation can be expressed as

$$-\nabla \cdot (D\nabla\Phi) + \sum_a \Phi = SourceTerm$$

where the Source term can be from a fixed source or a fission source expressed, respectively as

$$S_{indep.} \quad or \quad \frac{1}{k}\nu \sum_f \Phi$$

Using the Fick's law, expressed by

$$J = -D\nabla\Phi$$

Eq. (1) reduces to

$$\nabla J + \sum_a \Phi = \frac{1}{k}(\nu \sum_f)\Phi$$

To derive the finite-difference form of the diffusion equation Eq. (4) is integrated over discrete mesh volumes ($\Delta V_{i,j,k} = \Delta x_i \Delta y_{ji} \Delta z_k$), hence,

$$\Delta j \Delta k \int_{x_{ii}-1/2}^{x_i+1/2} dx \frac{dJ}{dx} + \Delta i \Delta k \int_{y_i-1/2}^{y_i+1/2} dy \frac{dJ}{dy} + \Delta j \Delta k \int_{z_i-1/2}^{z_i+1/2} dz \frac{dJ}{dz} + \int_V dV \, \Sigma_a \Phi = \int_V \frac{1}{k} (\nu \, \Sigma_f) \Phi$$

Eq. (5) can be rewritten in terms of the current entering/leaving a cell as

$$J\Big|_{x_i+1/2} - J\Big|_{x_i-1/2} + J\Big|_{y_i+1/2} - J\Big|_{y_i-1/2} + J\Big|_{z_{ii}+1/2} - J\Big|_{z_i-1/2} + \Sigma_a \int_V dV \, \Phi = \frac{1}{k} (\nu \, \Sigma_f) \int_V dV \, \Phi$$

The cell-averaged flux is given by

$$\overline{\Phi}_{ijk} = \frac{\int_V dV \, \Phi}{\int_{x-1/2}^{x+1/2} dx \int_{y-1/2}^{y+1/2} dy \int_{z-1/2}^{z+1/2} dz} = \frac{1}{\Delta x_i \Delta y_j \Delta z_k} \int_v dV \, \Phi$$

Using Eq. (7), Eq. (6) reduces to

$$J\Big|_{x_i+1/2} - J\Big|_{x_i-1/2} + J\Big|_{y_i+1/2} - J\Big|_{y_i-1/2} + J\Big|_{z_{ii}+1/2} - J\Big|_{z_i-1/2} + \Delta x_i \Delta y_j \Delta z_k \, \Sigma_a \, \overline{\Phi}_{ijk} = \frac{1}{k} \Delta x_i \Delta y_j \Delta z_k (\nu \, \Sigma_f) \overline{\Phi}_{ijk}$$

The current formulations are given by

$$J\big|_{m+1/2} = -2d_{m,m+1}(\Phi_{m+1} - \Phi_m)$$

$$where$$

$$d_{m,m+1} = 2\frac{d_m d_{m+1}}{d_m + d_{m+1}}$$

$$J\big|_{m-1/2} = -2d_{m-1,m}(\Phi_m - \Phi_{m-1})$$

$$where$$

$$d_{m-1,m} = 2\frac{d_m d_{m-1}}{d_m + d_{m-1}}$$

$$and$$

$$d_m = \frac{D_m}{\Delta_m} \qquad\qquad m = i, j, or\ k$$

Eq. (8) can be expressed in a matrix form as

$$\overline{\overline{A}} * \overline{\Phi} = \overline{Q}$$

Note that Eq. (10) includes a general boundary condition using an albedo coefficient. The derivation of boundary conditions is not presented here for brevity. Interested readers should consult Ref. (2). Using the above formulation we can arrange the coefficients into a banded diagonal matrix. The coefficient matrix, **A** takes the form seen in Figure 1. Using the Lower-Upper (LU) Decomposition approach the solution for the flux Φ is obtained.

$$\begin{bmatrix} a_{1,1,1} & a^{i}_{2,1,1} & \cdots & \cdots & a^{j}_{1,2,1} & \cdots & \cdots & \cdots & \cdots & \cdots & a^{k}_{1,1,2} & \cdots & \cdots \\ a^{i}_{2,1,1} & a_{2,1,1} & a^{i}_{3,1,1} & \cdots & \cdots & a^{j}_{1,2,1} & \cdots & \cdots & & a^{k}_{1,1,2} & \cdots & & \\ \vdots & \ddots & \ddots & \ddots & & \ddots & & & & \ddots & & & \\ \vdots & & & & & & & & & & & & \\ \cdots & a^{k}_{i,j,k-1} & \cdots & \cdots & a^{j}_{i,j-1,k} & \cdots & a^{i}_{i-1,j,k} & a_{i,j,k} & a^{i}_{i+1,j,k} & \cdots & a^{j}_{i,j+1,k} & \cdots & \cdots & a^{k}_{i,j,k+1} & \cdots \\ \vdots & & & & & & & & & & & & \\ \vdots & & \ddots & & & & \ddots & & & & \ddots & \ddots & \\ \cdots & \cdots & a^{k}_{I,J,K-1} & \cdots & \cdots & \cdots & a^{j}_{I,J-1,K} & \cdots & \cdots & \cdots & a^{i}_{I-1,J,K} & a_{I,J,K} \end{bmatrix}$$

Figure 1. Coefficient matrix form of the finite-difference neutron diffusion equations.

Eq. (10) can be used to solve two types of problems: fixed source and eigenvalue problems. This means that **Q** can either be equal to **S** (e.g. fixed source) or be equal to $\frac{1}{k}\overline{\overline{F}}\,\overline{\Phi}$ (e.g. fission source where $\overline{\overline{F}} = \overline{\overline{\nu\Sigma}}_{f}$).

In the case of a fission source the eigenvalue (k) and flux values must initially be guessed then iterations performed until the solution converges. The convergence criteria considered are:

$$\max\left|\frac{\Phi^{(m)}_{i,j,k} - \Phi^{(m-1)}_{i,j,k}}{\Phi^{(m-1)}_{i,j,k}}\right| < 10^{-4}$$

and

$$\left|\frac{k^{(m)} - k^{(m-1)}}{k^{(m-1)}}\right| < 10^{-6}$$

IMPLEMENTATION

The program SENDIFF was written in C++ and compiled using GNU v.3.3.5 g++ compiler. The source code contained matrix subroutines developed by the National Institute of Standards and Technology (NIST) known as Template Numerical Toolkit (TNT).[2]

The code reads the data from an input file and arranges the data into the aforementioned finite-difference formulations (Eq. 10). The output is then arranged into an ASCI data file that can be processed by TecPlot (a commercial graphics package, www.tecplot.com) for generation of a 3-D or 2-D graphical display. Also, the program output file contains data on computation time, eigenvalues, and geometric meshing.

The model used in the analysis of this program, shown in Figure 2, was a 6-cm cube of plutonium which, was placed inside a cardboard container, modeled as 60% density cellulose that was then placed inside an iron shipping container. Plutonium is a source of fast neutrons which could potentially be detected by radiation detectors. Dimensions of the problem are given in Table 1.

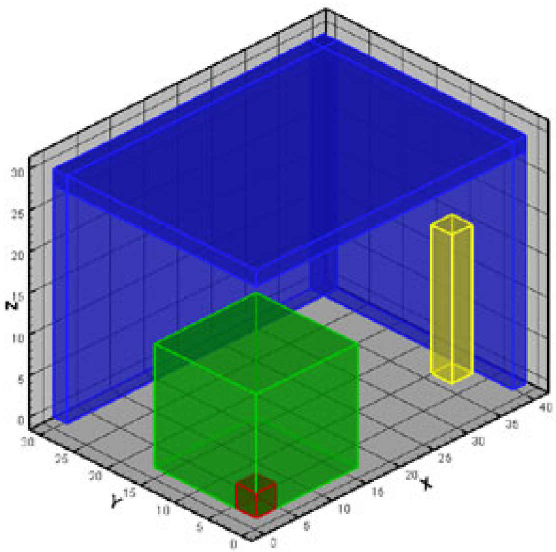

Figure 2. Description of the sample problem.

Table 1
Volume of Regions

Region	Volume (cm^3)
Plutonium	6 X 6 X 6
Cardboard Box	30 X 30 X 30
Shipping Container	80 X 60 X 60

The nuclear data including, diffusion coefficient, absorption and fission cross sections, are listed in Table 2. Note that here we only consider one energy group, because the current version of SENDIFF includes a one-group formulation.

Table 2
Nuclear Data for Materials

Material	D (cm)	-a (cm^{-1})	-f (cm^{-1})

Pu	1.12045×10^{0}	1.1825×10^{-1}	6.0421×10^{-1}
Box	8.66972×10^{0}	2.1743×10^{-3}	-
Air	4.12786×10^{6}	1.0641×10^{-8}	-
Fe	1.59352×10^{0}	1.2588×10^{-2}	-
He-3	2.83543×10^{3}	1.9912×10^{-5}	-

RESULTS

The sample problem was run on a 2.4 GHz Intel Xeon processor and the solution was obtained in 3946 s (approximately one hour and six minutes). The model included 7600 spatial meshes (25 in x, 16 in y, and 19 in z). Variable meshing techniques were used to place more meshes around the plutonium and less in the air volume, because the mean free path of neutrons inside the plutonium is much less than air. Since, this problem is an eigenvalue problem, (i.e. the source of neutrons originated from fission and fission depends on the neutron flux) iterations had to be performed. This model required 13 iterations.

Figure 3 shows the 3-D neutron flux distribution throughout the model, and Figure 4 shows x-y distribution at z=0. In both figures one can resolve most of the material regions. For example, the iron wall can be seen at the edge of the model. Figures 5 and 6 show 2-D flux distributions in logarithmic scale as a function of x for y=z=0cm and y=4cm and z=3cm, respectively. As expected, the maximum flux occurs at the plutonium cube and drops exponentially moving away from the cube. For example the flux at the He-3 detector is only 3.6% of the flux at the center of the plutonium cube. Further, the flux distribution shows minimal change within the air region, as expected.

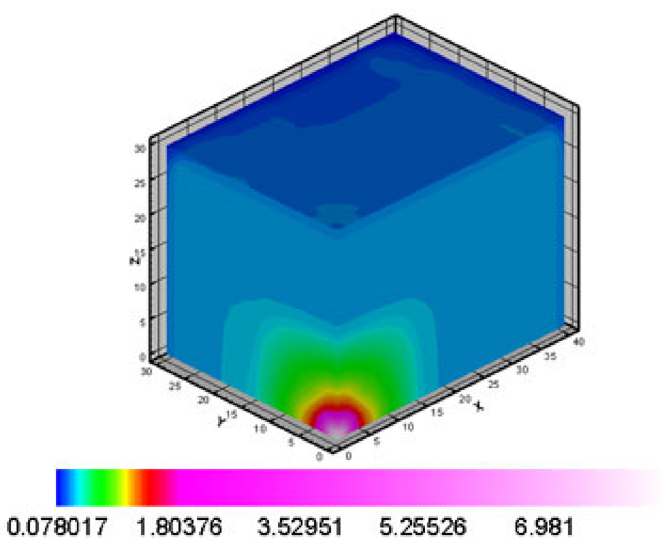

Figure 3. 3-D flux distribution throughout the sample problem

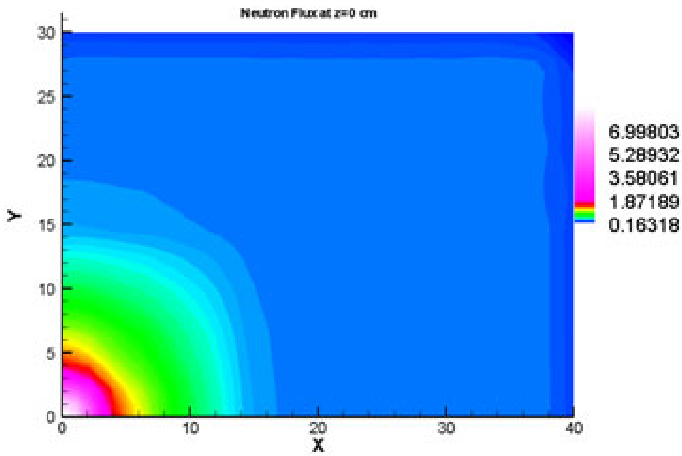

Figure 4. 2-D flux distribution at z=0

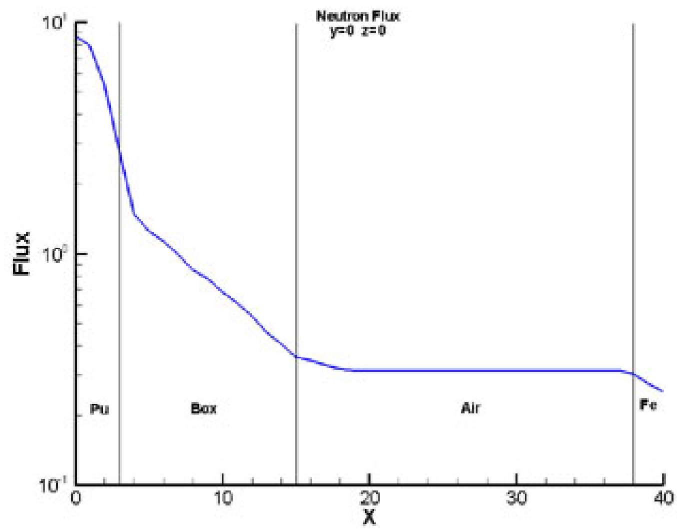

Figure 5. X-dependant flux distribution at y=z=0cm

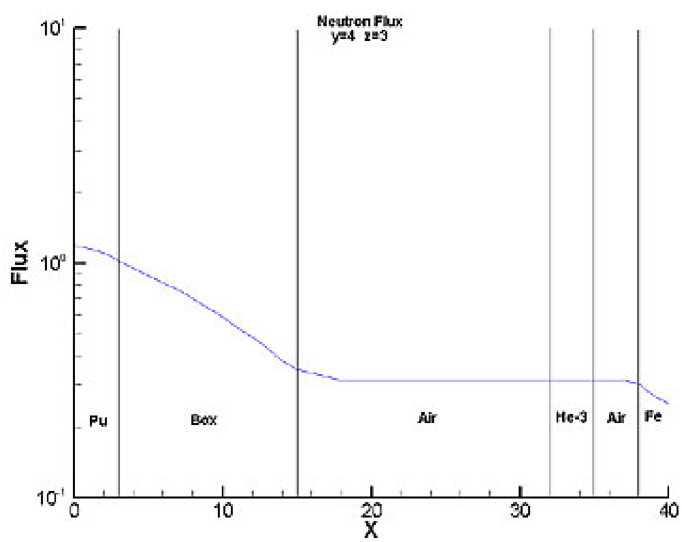

Figure 6. X-dependant flux distribution through at y=4cm, z=3cm.

The SENDIFF solution shows no change in flux through the He-3 detector. This means that the detector cannot detect the nuclear material of interest. This result has inherent uncertainty due to the one-group capabilities of SENDIFF; however, one can overcome this uncertainty if SENDIFF is to be extended to a multi-group formulation.

SUMMARY AND CONCLUSIONS

This project sought to model a realistic situation in which determining flux would be critical to developing detection methods for nuclear weapons material. The program SENDIFF provided flux distributions that are consistent with physical phenomenon. The flux behaved as expected in the different regions modeled in the problem.

One of the main drawbacks to the practicality of SENDIFF was its long computation time. To arrive at the solution to this problem, over one hour of computation time was required. In practice this would not be enough computation time reduction to warrant a diffusion approximation over a full transport calculation. However, techniques can be utilized such as compressed diagonal storage (CDS) to reduce the memory requirements by several orders of magnitude. Iterative matrix solution techniques could also be implemented instead of LU decomposition to reduce the number of mathematical operations necessary to solve the system of equations. Furthermore, this calculation was performed on a single processor. If the solution was implemented in a parallel computing environment with multiple processors, the computation time would be greatly reduced. Finally, the applicability of SENDIFF for practical problems could also be improved if multiple energy group considerations were included.

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