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TITLE: **AN EXPONENTIAL DISCONTINUOUS SCHEME FOR X-Y GEOMETRY TRANSPORT PROBLEMS**

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AN EXPONENTIAL DISCONTINUOUS SCHEME FOR X-Y-Z GEOMETRY TRANSPORT PROBLEMS

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ABSTRACT

The recently developed exponential discontinuous spatial differencing scheme for the discrete-ordinate equations has been extended to x-y-z geometry with hexahedral cells. This scheme produces strictly positive angular fluxes given positive discrete-ordinate sources. The exponential discontinuous scheme has been developed and implemented into the three-dimensional, discrete-ordinate code, THREEDANT. Numerical results are given which show that the exponential discontinuous scheme is very accurate for deep-penetration transport problems with optically thick spatial meshes.

I. INTRODUCTION

Recently, the algebraically equivalent nonlinear characteristic[1-3] (NC) and exponential characteristic[4-5] (EC) spatial differencing schemes were developed. These schemes use the method of characteristics with an exponential representation for the discrete-ordinate source within each spatial cell. This source representation is derived using information theory[6]. The NC/EC scheme is very accurate, especially for deep-penetration problems with optically thick spatial cells. The NC/EC scheme also produces strictly positive angular fluxes given positive discrete-ordinate sources. Recently we developed an exponential discontinuous (ED) scheme in x-y geometry based upon an exponential representation for the angular flux within each cell[7]. This representation is also derived using information theory. The motivation for the ED scheme is that it is much less complicated to derive and implement than the NC/EC scheme and is assumed to be considerably less computationally expensive in x-y-z geometry. The NC/EC scheme is exact for pure-absorbing problems in all Cartesian geometries. The ED scheme is only exact for pure-absorbing problems in slab geometry. Nonetheless, the ED scheme appears to be nearly as accurate as the NC/EC scheme for many problems and also produces strictly positive angular fluxes. The ED scheme has been extended to x-y-z geometry with a hexahedral mesh and has been implemented into the three-dimensional, discrete-ordinate code, THREEDANT™ [8].

The remainder of the paper will proceed as follows: in Sec. II, we derive the ED scheme in x-y-z geometry and discuss the method of solution; in Sec. III, we present some numerical results to show the accuracy and positivity of the ED scheme; and in Sec IV, we conclude with a discussion.

II. THE EXPONENTIAL DISCONTINUOUS SCHEME

The mono-energetic, x-y-z geometry discrete-ordinate equations are given by

$$\mu_m \frac{\partial}{\partial x}\psi_m(x,y,z) + \eta_m \frac{\partial}{\partial y}\psi_m(x,y,z) + \xi_m \frac{\partial}{\partial y}\psi_m(x,y,z) + \sigma_t(x,y,z)\psi_m(x,y,z) = S_m(x,y,z) \tag{1}$$

Here $\psi_m(x,y,z)$ is the discrete ordinate angular flux and $S_m(x,y,z)$ is the discrete ordinate source comprised of a combination of scattering, fission or fixed sources. We use a hexahedral mesh with each spatial cell having dimensions $x_{i-1/2} \le x \le x_{i+1/2}$, $y_{j-1/2} \le y \le y_{j+1/2}$, and $z_{k-1/2} \le z \le z_{k+1/2}$. We assume that the material properties are constant within each mesh cell.

We begin our derivation of the ED scheme by taking the zeroth, x, y and z spatial coordinate moments of Eq.(1). This is done by multiplying Eq.(1) by 1, $P_1(x) = 2(x - x_i)/\Delta x_i$, $P_1(y) = 2(y - y_j)/\Delta y_j$ and $P_1(z) = 2(z - z_k)/\Delta z_k$, and integrating over the volume of the cell. Here $\Delta x_i = x_{i+1/2} - x_{i-1/2}$, $x_i = (x_{i-1/2} + x_{i-1/2})/2$, $\Delta y_j = y_{j+1/2} - y_{j-1/2}$, $y_j = (y_{j+1/2} + y_{j-1/2})/2$, $\Delta z_k = z_{k+1/2} - z_{k-1/2}$, and $z_k = (z_{k+1/2} + z_{k-1/2})/2$. This gives the following four moment balance equations:

$$\frac{\mu_m}{\Delta x_i}\left(\psi_{m,i-1/2,j,k} - \psi_{m,i-1/2,j,k}\right) + \frac{\eta_m}{\Delta y_j}\left(\psi_{m,i,j+1/2,k} - \psi_{m,i,j-1/2,k}\right) + \frac{\xi_m}{\Delta z_k}\left(\psi_{m,i,j,k+1/2} - \psi_{m,i,j,k-1/2}\right) + \sigma_{t,i,j,k}\psi_{m,i,j,k} = S_{m,i,j,k} \tag{2}$$

$$\frac{3\mu_m}{\Delta x_i}\left(\psi_{m,i+1/2,j,k} + \psi_{m,i-1/2,j,k} - 2\psi_{m,i,j,k}\right) + \frac{\eta_m}{\Delta y_j}\left(\psi^x_{m,i,j+1/2,k} - \psi^x_{m,i,j-1/2,k}\right) + \frac{\xi_m}{\Delta z_k}\left(\psi^x_{m,i,j,k+1/2} - \psi^x_{m,i,j,k-1/2}\right) + \sigma_{t,i,j,k}\psi^x_{m,i,j,k} = S^x_{m,i,j,k} \tag{3}$$

$$\frac{\mu_m}{\Delta x_i}\left(\psi^y_{m,i+1/2,j,k} - \psi^y_{m,ii-1/2,j,k}\right) + \frac{3\eta_m}{\Delta y_i}\left(\psi_{m,i,j+1/2,k} + \psi_{m,i,j-1/2,k} - 2\psi_{m,i,j,k}\right) + \frac{\xi_m}{\Delta z_k}\left(\psi^y_{m,i,j,k+1/2} - \psi^y_{m,i,j,k-1/2}\right) + \sigma_{t,i,j,k}\psi^y_{m,i,j,k} = S^y_{m,i,j,k} \tag{4}$$

$$\frac{\mu_m}{\Delta x_i}\left(\psi^z_{m,i+1/2,j,k} - \psi^z_{m,i-1/2,j,k}\right) + \frac{\eta_m}{\Delta y_i}\left(\psi^z_{m,i,j+1/2,k} - \psi^z_{m,i,j-1/2,k}\right) + \frac{3\xi_m}{\Delta z_k}\left(\psi_{m,i,j,k+1/2} + \psi_{m,i,j,k-1/2} - 2\psi_{m,i,j,k}\right) + \sigma_{t,i,j,k}\psi^z_{m,i,j,k} = S^z_{m,i,j,k} \tag{5}$$

where,

$$\psi_{m,i,j,k} \equiv \frac{1}{\Delta x_i \Delta y_j \Delta z_k} \int_{x_{i+1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{z_{k+1/2}}^{z_{k+1/2}} \psi_m(x,y,z)dxdydz, \tag{6}$$

and

$$\psi^n_{m,i,j,k} \equiv \frac{3}{\Delta x_i \Delta y_j \Delta z_k} \int_{x_{i+1/2}}^{x_{i+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{z_{k+1/2}}^{z_{k-1/2}} P_1(n)\psi_m(x,y,z)dzdydx, \quad n = x,y,z \ . \tag{7a-7c}$$

The definitions for the source moments are obtained by replacing ψ with S in Eqs. (6)-(7). The average and first spatial angular fluxes moments on the outgoing faces are defined as:

$$\psi_{m,i+1/2,j,k} \equiv \frac{1}{\Delta y_j \Delta z_k} \int_{y_{j-1/2}}^{y_{j-1/2}} \int_{z_{k+1/2}}^{z_{k+1/2}} \psi_m(x_{i+1/2},y,z)dzdy, \tag{8}$$

$$\psi^n_{m,i+1/2,j,k} \equiv \frac{1}{\Delta y_j \Delta z_k} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{z_{k+1/2}}^{z_{k+1/2}} P_1(n)\psi_m(x_{i+1/2},y,z)dzdy, \quad n = y,z, \tag{9a-9b}$$

$$\psi_{m,i,j+1/2,k} \equiv \frac{1}{\Delta x_i \Delta z_k} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{z_{k+1/2}}^{z_{k+1/2}} \psi_m(x,y_{j+1/2},z)dzdx, \tag{10}$$

$$\psi^n_{m,i,j+1/2,k} \equiv \frac{1}{\Delta x_i \Delta z_k} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{z_{k-1/2}}^{z_{k-1/2}} P_1(n)\psi_m(x,y_{j+1/2},z)dzdx, \quad n = x,z, \tag{11a-11b}$$

$$\psi_{m,j,k+1/2} \equiv \frac{1}{\Delta y_j \Delta x_i} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i+1/2}}^{x_{i+1/2}} \psi_m(x,y,z_{k+1/2})dxdy, \tag{12}$$

$$\psi^n_{m,i,j,k+1/2} \equiv \frac{1}{\Delta y_j \Delta x_i} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i+1/2}}^{x_{i+1/2}} P_1(n)\psi_m(x,y,z_{k+1/2})dxdy, \quad n = y,x. \tag{13a-13b}$$

At this point, we have four equations with thirteen unknowns. To obtain the auxiliary equations we assume an exponential representation for the angular flux within each cell. Using information theory[6], we find that this representation is given by

$$\psi_m(x,y,z) = a_{m,i,j,k} e^{\lambda^x_{m,i,j,k}P_1(x)+\lambda^y_{m,i,j,k}P_1(y)+\lambda^z_{m,i,j,k}P_1(z)} \ . \tag{14}$$

To find $a_{m,i,j,k}$, $\lambda^x_{m,i,j,k}$, $\lambda^y_{m,i,j,k}$ and $\lambda^z_{m,i,j,k}$, we apply our definitions for the zeroth, x, y and z spatial moments of the angular flux. Inserting Eq.(14) into Eqs.(6) - (7), we obtain

$$a_{m,i,j,k} = \psi_{m,i,j,k} \frac{\lambda^x_{m,i,j,k}}{sinh\left(\lambda^x_{m,i,j,k}\right)} \frac{\lambda^y_{m,i,j,k}}{sinh\left(\lambda^y_{m,i,j,k}\right)} \frac{\lambda^z_{m,i,j,k}}{sinh\left(\lambda^z_{m,i,j,k}\right)}, \tag{15}$$

and

$$\frac{\psi^n_{m,i,j,k}}{\psi_{m,i,j,k}} = 3\left[coth\left(\lambda^n_{m,i,j,k}\right) - \frac{1}{\lambda^n_{m,i,j,k}}\right], \quad n = x, y, z. \tag{16a-16c}$$

Next, we use Eq.(14) to obtain our auxiliary equations. We assume that the angular fluxes are discontinuous at the edges of the cell. Inserting Eq.(14) into Eqs.(8) to (13) gives the following nine auxiliary equations:

$$\psi_{m,i\pm1/2,j,k} = \psi_{m,i,j,k} \frac{\lambda^x_{m,i,j,k}}{sinh\left(\lambda^x_{m,i,j,k}\right)} e^{\pm\lambda^x_{m,i,j,k}}, \quad \mu_{m<} \gtrless 0, \tag{18}$$

$$\psi^n_{m,i\pm1/2,j,k} = \psi_{m,i,j,k} 3\left[coth\left(\lambda^n_{m,i,j,k}\right) - \frac{1}{\lambda^n_{m,i,j,k}}\right] \frac{\lambda^x_{m,i,j,k}}{sinh\left(\lambda^x_{m,i,j,k}\right)} e^{\pm\lambda^x_{m,i,j,k}}, \quad n = y, z, \quad \mu_{m<} \gtrless 0, \tag{19a-19b}$$

$$\psi_{m,i,j\pm1/2,k} = \psi_{m,i,j,k} \frac{\lambda^y_{m,i,j,k}}{sinh\left(\lambda^y_{m,i,j,k}\right)} e^{\pm\lambda^y_{m,i,j,k}}, \quad \eta_{m<} \gtrless 0, \tag{20}$$

$$\psi^n_{m,i\pm1/2,j,k} = \psi_{m,i,j,k} 3\left[coth\left(\lambda^n_{m,i,j,k}\right) - \frac{1}{\lambda^n_{m,i,j,k}}\right] \frac{\lambda^y_{m,i,j,k}}{sinh\left(\lambda^y_{m,i,j,k}\right)} e^{\pm\lambda^y_{m,i,j,k}}, \quad n = x, z, \quad \eta_{m<} \gtrless 0, \tag{21a-21b}$$

$$\psi_{m,i,j,k\pm1/2} = \psi_{m,i,j,k} \frac{\lambda^z_{m,i,j,k}}{sinh\left(\lambda^z_{m,i,j,k}\right)} e^{\pm\lambda^z_{m,i,j,k}}, \quad \xi_{m<} \gtrless 0, \tag{22}$$

$$\psi^n_{m,i,j,k\pm1/2} = \psi_{m,i,j,k} 3\left[coth\left(\lambda^n_{m,i,j,k}\right) - \frac{1}{\lambda^n_{m,i,j,k}}\right] \frac{\lambda^z_{m,i,j,k}}{sinh\left(\lambda^z_{m,i,j,k}\right)} e^{\pm\lambda^z_{m,i,j,k}}, \quad n = x, y, \quad \xi_{m<} \gtrless 0. \tag{23a-23b}$$

To summarize, the ED equations are given by Eq.(2)-(5),(16) and (18)-(23).

The ED equations are solved somewhat differently than existing linear differencing schemes since it is inherently nonlinear. As with most discrete-ordinates schemes, we use source-iteration (SI) to iteratively solve for the scattering source. However, for within cell calculations, the ED equations are solved using Newton-Raphson iterations for the cell average scalar fluxes and moments and the scalar fluxes and

moments on the outgoing faces. All within cell Newton-Raphson iterations are initialized with $\lambda_x, \lambda_y, \lambda_z = 0$, which from practical experience appears to be the most robust. Current studies are ongoing to obtain a diffusion accelerated solution method for the ED scheme. This has been done in slab geometry but has not been extended to multidimensional geometries.

Having coded the ED scheme and solution method, we encountered difficulties with problems with anisotropic scattering, when the truncated Legendre expansion of the discrete-ordinate source leads to negative sources. In order for a solution to be possible, the ED scheme requires that the solution be positive everywhere or negative everywhere. This results from information theory (maximum entropy). Therefore, it appears that solutions to the ED scheme can only be obtained if the scattering source is positive everywhere in the problem. Current investigations are ongoing to obtain positive discrete-ordinate sources regardless of the Legendre expansion of the scattering source.

III. Numerical Results

In this section we provide results for one test problem We compare the ED scheme with the linear discontinuous (LD), constant-linear nodal with negative flux fix-up (CLN/F) and adaptive weighted diamond difference (AWDD) schemes. The LD scheme does not use any negative flux fixup method. We cannot compare with the NC/EC scheme since it has not been developed and implemented in x-y-z geometry with hexahedral meshes.

The physical problem is a 120-cm cube of an iron alloy, in which is centered a 119-cm cube of an aqueous solution, in which is centered a 40-cm cube of the iron alloy, in which is centered a 10-cm cube of the aqueous solution that contains the source. Symmetry allows us to consider only one octant (a 60-cm cube) with reflecting boundaries on the bottom, left and front sides and vacuum boundaries on the top, right and back sides. The source emits 73.9 % of its neutrons in the first of three energy groups, with the remaining 26.1 % in the second energy group. We use an S_4 quadrature set and isotropic scattering cross sections. The cross sections for the aqueous solution are given in Table 1 and the cross section for the iron alloy are given in Table 2. All calculations are converged to a relative error of 10^{-3}.

In Figures 1 to 3 we present some results for the this test problem. Here, for each energy group, the scalar flux is given, for various mesh sizes, at a detector located at $59.5 \text{ cm} \le x \le 60.0 \text{ cm}$, $59.5 \text{ cm} \le y \le 60.0 \text{ cm}$, and $59.5 \text{ cm} \le z \le 60.0 \text{ cm}$. The coarsest mesh is 5 x 5 x 5 (5 cells along each spatial axis) and the finest mesh is 57 x 57 x 57. If a data point representing the solution for a given scheme at a given mesh does not appear on the graph, then it lies outside the domain of the graph or was a negative value. Negative solutions only appeared for the LD scheme. We observe that the ED scheme is far more accurate than the other schemes especially at the coarse meshes. Obtaining accurate fluxes at such localized locations is much more difficult that an integral quantity, such as the total leakage, especially in a deep-penetration problem such as this. We note that the ED scheme did not generate any negative fluxes. We also note that the error in the ED solution was never more than a factor of two for the coarsest meshes; all other scheme were off by several orders of magnitude at the coarsest meshes. Also, the AWDD scheme is not monotonically converging at the refined meshes.

For this problem the ED scheme took, on average, 4 times longer than the CLN/F scheme and 10 times longer than the AWDD on a per cell, per angle basis. Timing comparisons were not made with the LD scheme, since the implementation is not optimized for accurate comparisons.

IV. DISCUSSION

We have extended the ED scheme to x-y-z geometry with hexahedral meshes and implemented it into the THREEDANT^{TM} code. One of the main advantages of the ED scheme is that it produces strictly positive angular fluxes. We have tested the scheme on a variety of problems, including the one in this paper, and have found that it is very accurate for deep-penetration problems with optically thick spatial meshes.

We are in the process of extending the ED scheme to x-y-z geometry with unstructured tetrahedral meshes.

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Table 1: Cross Section Data for Aqueous Solution

Group Number (g)	$\sigma_{t,g}$	$\sigma_{s,g\to g}$	$\sigma_{s,(g-1)\to g}$
1	0.2656	0.1600	0.0000
2	1.1745	0.8220	0.1052
3	3.2759	2.2980	0.0730

Table 2: Cross Section Data for Iron Alloy

Group Number (g)	$\sigma_{t,g}$	$\sigma_{s,g\to g}$	$\sigma_{s,(g-1)\to g}$
1	0.2163	0.1760	0.0000
2	0.3255	0.2500	0.0399
3	1.1228	0.7982	0.0001

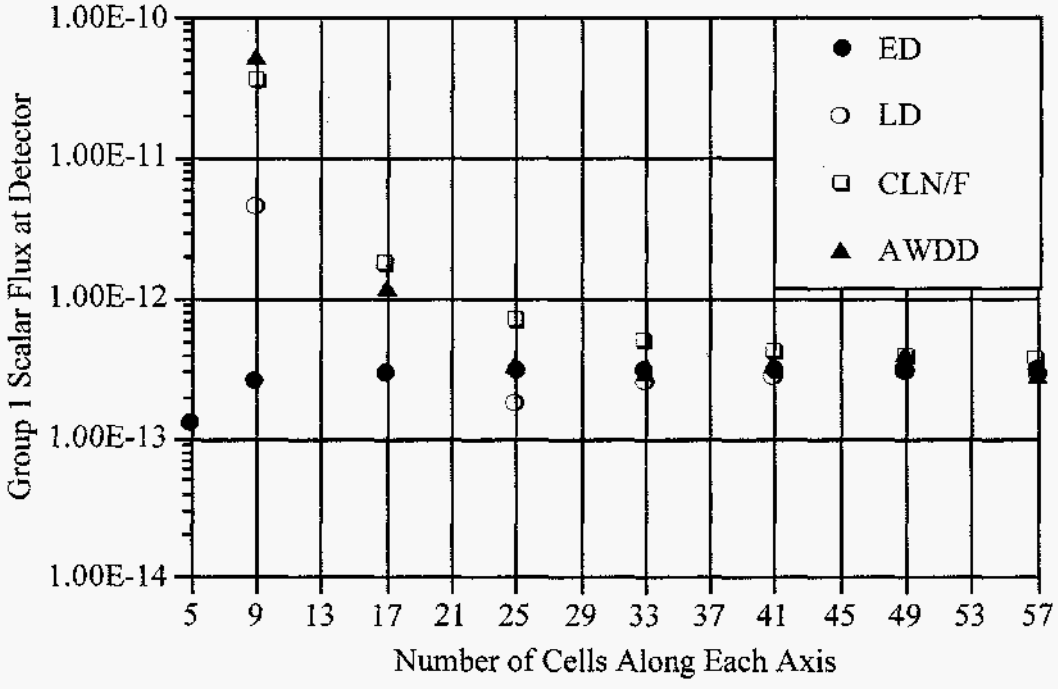

Figure 1: Group 1 Scalar Fluxes at the Detector Location

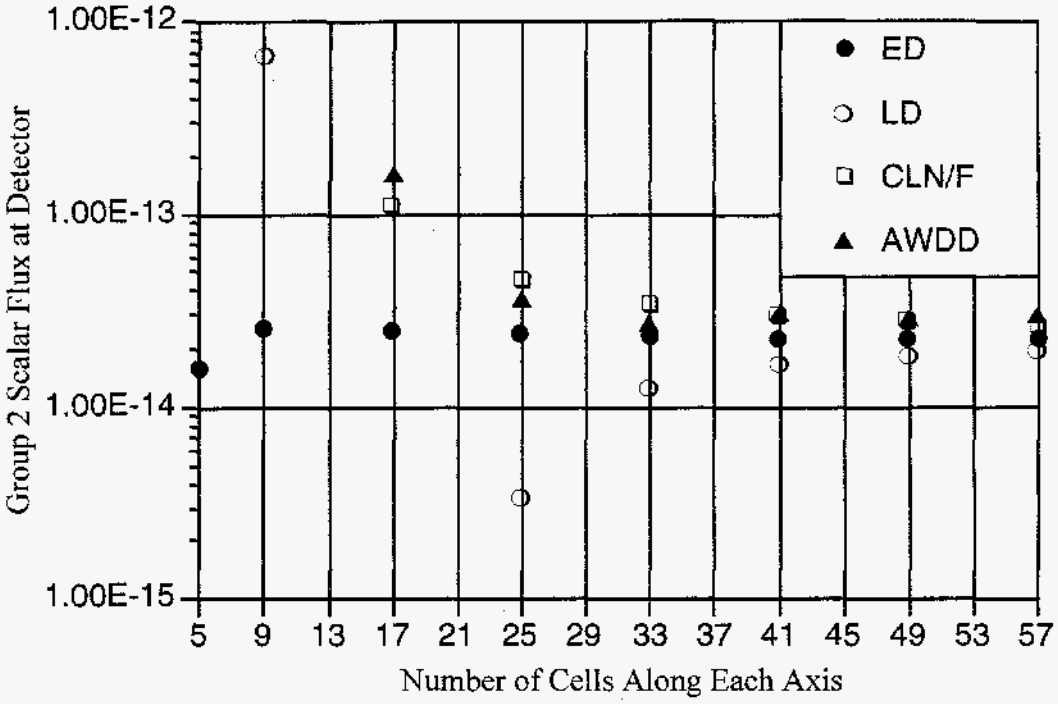

Figure 2: Group 2 Scalar Fluxes at the Detector Location

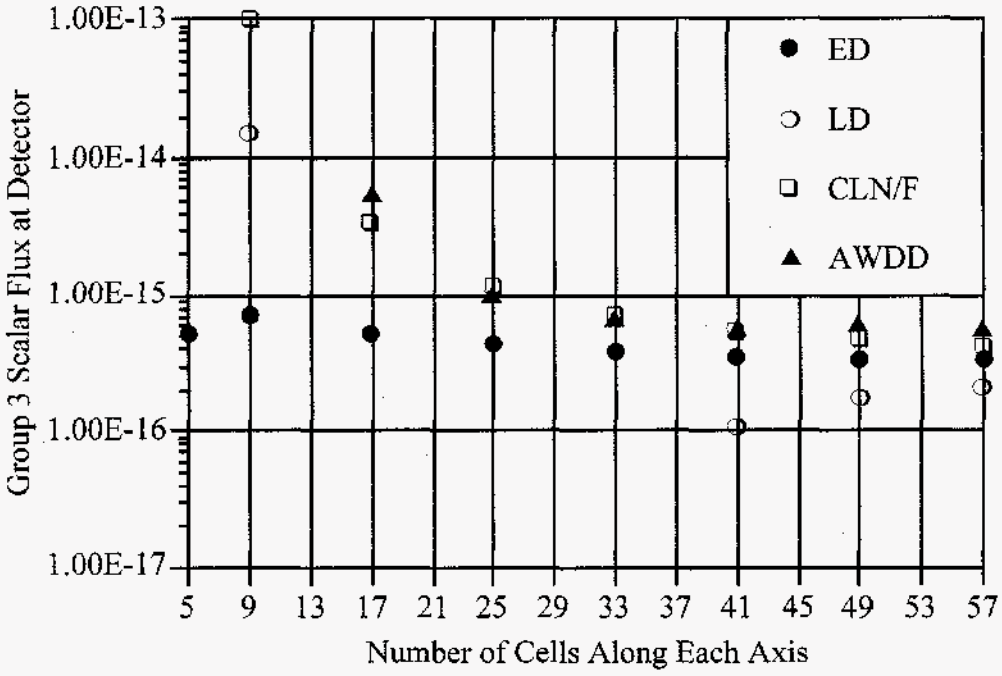

Figure 3: Group 3 Scalar Fluxes at the Detector Location