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ON EQUILATERAL TRIANGULAR MESHES

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THE TLC SCHEME FOR NUMERICAL SOLUTION OF THE TRANSPORT EQUATION
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Abstract

A new triangular linear characteristic TLC scheme for numerically solving the transport equation on equilateral triangular meshes has been developed. This scheme uses the analytic solution of the transport equation in the triangle as its basis. The data on edges of the triangle are assumed linear as is the source representation. A characteristic approach or nodal approach is used to obtain the analytic solution. Test problems indicate that the new TLC is superior to the widely used DITRI scheme for a accuracy and positively.

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THE TLC SCHEME FOR NUMERICAL SOLUTION OF THE TRANSPORT EQUATION ON EQUILATERAL TRIANGULAR MESHES

INTRODUCTION

An accurate difference scheme has been developed for solving the discrete- S_N form of the Boltzmann transport equation in equilateral-triangular meshes. This scheme will be referred to as the triangular linear characteristic scheme, TLC. In this scheme the source within each triangle is assumed to be linear in x and y ; and the data along the inflow faces is also assumed to be linear, hence the name "linear" characteristic. With this source and inflow information, it is possible to determine the exact analytic solution for the triangle. Using this analytic solution, it is possible to construct the cell average angular flux, the average angular flux on all outflow faces, and the first moment of the angular flux on all outflow faces. Of course, there are two sets of these expressions. One is for inflow through one face of a triangle and the other is for inflow through two faces.

For flow through one face the method of characteristics will be used to find the analytic solution. The technique is similar to that used in Reference 1 for rectangular x,y geometry. Flow through two faces a nodal method will be used to determine the analytic solution. This nodal method is similar to that used in Reference 2 for rectangular x,y geometry. For inflow through one face the angular flux of the vertex opposite the inflow face is also determined.

The TLC scheme is compared to the Diamond Triangular (DITRI) scheme^{3,4} by analyzing two test problems. The DITRI scheme is used in two discrete-ordinate transport codes which allow equilateral triangular meshes.^{5,6} In addition E. E. Lewis has recently modified the DIF3D code⁷ to use the DITRI scheme.

PRELIMINARIES

The TLC method is derived by solving the neutron transport equation analytically in an equilateral triangular domain. The boundary data and the source within each triangle are both assumed to be linear; hence, the word linear in TLC. In this section the notation, coordinate systems, source representations, and certain flux representations are introduced.

The notation used throughout this paper is

ψ is the angular flux;

ϕ is the scalar flux;

S is a source;

θ is the average first moment of the angular flux on some face of the triangle.

μ and η are the x - and y -direction direction cosines.

L , R , B , T , and A are subscripts such that L = left, R = right, B = bottom, and A = average. x , y , t , and s subscripts are used to denote the cell average x , y , t or s moment of a quantity. The subscript m is used to denote a discrete-ordinate direction.

In the (s,t) system the representation is

$$S(s,t) = S_A + \frac{2s}{\ell} S_s + \frac{3}{2h} (t - \frac{2h}{3}) S_t .$$

Later in the paper certain approximations will be developed for the source moments S_x , S_y , S_s , and S_t .

INFLOW THROUGH TWO FACES

In this section the analytic solution will be obtained by a method directly related to the nodal method used in (x,y) geometry. Using the (s,t) coordinate system the transport equation will be integrated over the s coordinate yielding an equation in t alone. The analytic solution to this equation is indicated and the expression for the average outflow angular flux ψ_R is determined. Using a similar technique the average outflow angular first flux moment θ_R is determined. Since there are no unknown transverse leakage terms in these equations, the result is exactly the same as would have been obtained using the method of characteristics to determine the solution. This statement has been verified by solving the transport equation using the method of characteristics. The nodal form is used here because it yields a more convenient form for making approximations to θ_R .

Let us assume that

$$\mu, \eta > 0, \quad \text{and}$$

$$0 \leq \tan^{-1} \left(\frac{\eta}{\mu} \right) \leq \frac{\pi}{3} .$$

For these conditions the triangle in Figure 1 has inflow through the bottom and left faces. The angular flux representations

$$\psi_B (t/\sqrt{3}, t) = \psi_B + \frac{2}{h} (t - \frac{h}{2}) \theta_B ,$$

and

$$\psi_L (-t/\sqrt{3}, t) = \psi_L + \frac{2}{h} (t - \frac{h}{2}) \theta_L ,$$

are known. The average angular flux ψ_R and first moment θ_R are to be determined. Note that

$$\psi_R (s, h) = \psi_P - \frac{2s}{\ell} \theta_R .$$

In Figure 1 an equilateral triangle is shown with (x,y) and (s,t) coordinate systems indicated. The (s,t) coordinate system is obtained by a clockwise rotation of θ with respect to the (x,y) axes.

In the (x,y) system, the transport equation is

$$\mu_m \frac{\partial \psi_m}{\partial x} + \eta_m \frac{\partial \psi_m}{\partial y} + \sigma \psi_m(x,y) = S_m(x,y) \quad (1a)$$

In the (s,t) system,

$$\mu'_m \frac{\partial \psi_m}{\partial s} + \eta'_m \frac{\partial \psi_m}{\partial t} + \sigma \psi_m(s,t) = S_m(s,t) \quad (1b)$$

From this point on the discrete-ordinates subscript m will be suppressed. Here,

$$\mu' = \frac{\mu - \eta\sqrt{3}}{2} \quad ,$$

$$\eta' = \frac{\sqrt{3}\mu + \eta}{2} \quad ,$$

and σ is the total cross section.

The data along the faces of the triangle in Figure 1 is assumed to be linear. That is,

$$\psi_L = \psi_L + \left[\frac{2y}{h} - 1 \right] \theta_L \quad ,$$

$$\psi_B = \psi_B + \left[\frac{2x}{\ell} - 1 \right] \theta_B \quad , \quad \text{and}$$

$$\psi_R = \psi_R + \left[\frac{2y}{h} - 1 \right] \theta_R \quad ,$$

where ℓ is the length of a side of the triangle and h is the altitude of the triangle ($h = \frac{\sqrt{3}}{2} \ell$). A linear moment representation is assumed for the source in the triangle. In the (x,y) system,

$$S(x,y) = S_A + \frac{2}{\ell} \left(x - \frac{\ell}{2} \right) S_x + \frac{3}{2h} \left(y - \frac{h}{3} \right) S_y \quad .$$

We now operate on the transport equation in the (s,t) system, Eq. (1b), with the operator

$$\frac{\sqrt{3}}{2t} \int_{-t/\sqrt{3}}^{t/\sqrt{3}} ds \quad .$$

After using Leibnitz rule for the derivative of an integral, we obtain the equation

$$\begin{aligned} \frac{d}{dt} \psi^0(t) + \psi^0(t) \left[\frac{1}{t} + \frac{\sigma}{\eta'} \right] &= \frac{1}{2t} [\psi_B(t/\sqrt{3}, t) + \psi_L(-t/\sqrt{3}, t)] \\ - \frac{h'}{\eta' t} \cdot [\psi_B(t/\sqrt{3}, t) - \psi_L(-t/\sqrt{3}, t)] &+ \frac{1}{\eta'} \cdot [S_A - S_t] + \frac{t}{\eta'} \cdot \frac{3}{2h} S_t \quad . \end{aligned} \quad (2)$$

Here,

$$\psi^0(t) = \frac{\sqrt{3}}{2t} \int_{-t/\sqrt{3}}^{t/\sqrt{3}} \psi(s, t) ds \quad .$$

The solution to Eq. (2) is

$$\begin{aligned} \psi^0(t=h) &= \psi_R = \rho' P_0 \psi_B + (1 - \rho') P_0 \psi_L \\ &+ \rho' \theta_B (2P_1 - P_0) + (1 - \rho') \theta_L (2P_1 - P_0) \\ &+ \frac{(3P_2 - 2P_1)h}{2\eta'} S_t + \frac{P_1 h}{\eta'} S_A \quad . \end{aligned} \quad (4)$$

The neutron balance equation for this triangle is

$$\frac{2\eta'}{l} (\psi_R - \psi_L) + \frac{\eta'}{h} [2\psi_T - \psi_R - \psi_L] + \sigma \psi_A = S_A \quad . \quad (5)$$

Substituting the expression for ψ_R into the balance equation, the following result is obtained for the cell-average angular flux as a function of inflow quantities.

$$\begin{aligned} \psi_A &= 2P_1 [(1 - \rho') \psi_L + \rho' \psi_B] \\ &- 2(P_1 - P_2) [(1 - \rho') \theta_L + \rho' \theta_B] + \frac{S_A h P_2}{\eta'} + \frac{(P_3 - P_2)h}{\eta'} S_t \quad . \end{aligned} \quad (6)$$

Here,

$$\rho' = 0.5 (1 - \sqrt{3} \mu' / \eta') \quad ,$$

$$\varepsilon' = \sigma h / \eta' \quad ,$$

$$P_0(\varepsilon') = (1 - e^{-\varepsilon'}) / \varepsilon' \quad , \quad P_0(0) = 1 \quad ,$$

$$P_1(\varepsilon') = (1 - P_0) / \varepsilon' \quad , \quad P_1(0) = 1/2 \quad ,$$

$$P_2(\varepsilon') = (1 - 2P_1) / \varepsilon' \quad , \quad P_2(0) = 1/3 \quad ,$$

$$P_3(\varepsilon') = (1 - 3P_2) / \varepsilon' \quad , \quad P_3(0) = 1/4 \quad .$$

As $\sigma \rightarrow 0$, $\varepsilon' \rightarrow 0$ and the functions P_0 , P_1 , P_2 , and P_3 tend to the finite values indicated above.

Now to obtain an expression for θ_R we operate on the transport equation with

$$\frac{9}{2t^2} \int_{-t/\sqrt{3}}^{t/\sqrt{3}} s \, ds \quad ; \quad \text{define } \psi_s^1(t) \equiv \frac{9}{2t^2} \int_{-t/\sqrt{3}}^{t/\sqrt{3}} \Psi(s,t) s \, ds \quad .$$

Once again using Leibnitz rule for the derivative of an integral, we obtain

$$\begin{aligned} & \frac{d\psi_s^1(t)}{dt} + \psi_s^1(t) \left[\frac{2}{t} + \frac{\sigma}{\eta'} \right] \\ &= \frac{t}{h} S_s + \frac{3\sqrt{3}}{2t} \frac{\mu'}{\eta'} [2\psi^0(t) - \Psi_B(t/\sqrt{3}, t) - \Psi_L(-t/\sqrt{3}, t)] + \frac{3}{2t} [\Psi_B(t/\sqrt{3}, t) \\ & \quad - \Psi_L(-t/\sqrt{3}, t)] \quad . \end{aligned} \tag{7}$$

The solution to Eq. (7) is

$$\begin{aligned}
\psi_s^1(t = h) = -\theta_R &= \frac{S_s h \cdot P3}{\eta'} \\
&+ \frac{3\sqrt{3}}{2} \cdot P1 \cdot \frac{\mu'}{\eta'} [2(\psi_A - \psi_t) - (\psi_B - \theta_B) - (\psi_L - \theta_L)] \\
&+ 3\sqrt{3} \cdot P2 \cdot \frac{\mu'}{\eta'} \left[\frac{3}{2} \psi_t - (\theta_B + \theta_L) \right] + \frac{3 \cdot P1}{2} (\psi_B - \theta_B) - (\psi_L - \theta_L) \\
&+ 3 \cdot P2 \cdot [\theta_B - \theta_L] \quad . \quad (8)
\end{aligned}$$

Using the approximation

$$\psi_t \approx \psi_R - \psi_A$$

for the average first moment, the expression for θ_R becomes

$$\begin{aligned}
-\theta_R &= \frac{S_s h P3}{\eta'} + 9\psi_A (1 - 2\rho') (P1 - P2) \\
&+ 3P1 [\rho' \psi_B + (1 - \rho') \psi_L] + 3(2P2 - P1) [\rho' \theta_B - (1 - \rho') \theta_L] \\
&+ 3\psi_R (1 - 2\rho') (3P2 - 2P1) \quad . \quad (9)
\end{aligned}$$

Now the equations for ψ_R , ψ_A , and θ_R have well-defined values as $\sigma \rightarrow 0$. If the cross section and the source terms in these equations are set to zero, it can be shown from geometric arguments that the resulting equations exhibit the correct behavior for streaming in a void.

INFLOW THROUGH ONE FACE

The case of inflow through one face of the triangle in Figure 1 will now be considered. In this case

$$\frac{2\pi}{3} \geq \tan^{-1} \frac{n}{\mu} \geq \frac{\pi}{3} \quad .$$

ψ_R , ψ_L , θ_R and θ_L must be determined.

The transport equation, Equation (1a), can be written in operator form as

$$L\Psi(x, y) = S(x, y) \quad .$$

The solution of the transport equation can be written

$$\Psi(x,y) = X(x,y) + a + bx + cy \quad (10)$$

Using the linear representation for the source $S(x,y)$ we find ,

$$c = \frac{3}{2\sigma h} S_y \quad , \quad b = \frac{2}{\sigma \ell} S_x \quad ,$$

$$a = \frac{1}{\sigma} (S_A - S_x - \frac{S_y}{2}) - \frac{\mu}{\sigma} b - \frac{\eta}{\sigma} c \quad .$$

Now $X(x,y)$ is the solution of the equation

$$LX = 0 \quad .$$

Using the method of characteristics the solution everywhere inside and on the surface of the triangle is

$$X(x,y) = \left[\chi_B - \left(1 - \frac{2x}{\ell} + \frac{2\mu y}{n\ell}\right) \beta_B \right] e^{-\sigma y/\eta} \quad (11)$$

Here χ_B and β_B are the average value of X and its first moment on the inflow (bottom) face such that

$$X(x, y = 0) = \chi_B + \beta_B \left(\frac{2x}{\ell} - 1 \right) \quad (12)$$

The average values of X along the left and right faces are then

$$\chi_L = P_0(\chi_B - \beta_B) + 2\beta_B \rho (P_0 - P_1) \quad (13)$$

and

$$\chi_R = P_0(\chi_B + \beta_B) - 2\beta_B(1 - \rho) (P_0 - P_1) \quad (14)$$

With these results, we can use the transformation, Eq. (10), to obtain expressions for the average value of the angular flux along the left and right faces of the triangle. On the left face

$$\psi_L = P_0(\psi_B - \theta_B) + 2\rho\theta_B (P_0 - P_1)$$

$$+ \frac{h}{\eta} S_A P_1 + \frac{h}{2\eta} S_x [P_2(1 - 4\rho) - 2P_1(1 - 2\rho)] + \frac{S_y h}{4\eta} (3P_2 - 2P_1) \quad (15)$$

The average angular outflow flux through the right face is

$$\psi_R = \psi_L + 2P1\theta_B + \frac{S_x P2h}{\eta} \quad (16)$$

The cell-average angular flux is

$$\begin{aligned} \psi_A = & 2P1 \psi_B + 2\theta_B (1 - 2\rho)(P2 - P1) + S_A P2 \frac{h}{\eta} + \frac{S_x h}{\eta} (P3 - P2)(1 - 2\rho) \\ & + \frac{S_y h}{2\eta} (P3 - P2) \quad (17) \end{aligned}$$

In this section

$$\rho = 0.5(1 - \sqrt{3} \mu/\eta) \quad , \quad \text{and } \varepsilon = \sigma h/\eta$$

The P0, P1, P2, and P3 are as defined following Eq. (3) with ε' replaced by ε .

Since the singular characteristic does not intersect either of the outflow faces, the analytic angular flux solution is continuous along these faces. Since this is the case, we make the simple approximations

$$\theta_T = (\psi_3 - \psi_L + \theta_L)/2 \quad , \quad (18)$$

and

$$\theta_R = (\psi_3 - \psi_L - \theta_L)/2 \quad , \quad (19)$$

for the first moments on the outflow faces. This approximation has been used with good results in rectangular meshes for the one outflow face upon which the analytic angular flux solution is continuous. The angular flux at the point 3 in the triangle is given by

$$\begin{aligned} \psi_3 = & [\psi_B - (1 - 2\rho) \theta_B] e^{-\varepsilon} \\ & + \frac{S_A h}{\eta} P0 + (1 - 2\rho) S_x (P1 - P0) \frac{h}{\eta} + \frac{S_y h}{2\eta} (3P1 - P0) \quad (20) \end{aligned}$$

When the direction of neutron flow is parallel to the left face of the triangle [$\tan^{-1}(\eta/\mu) = \pi/3$] Equation (4) for ψ_R should yield the same result as Equation (16) for ψ_R . This does occur. For $\tan^{-1}(\eta/\mu) = \pi/3$, $\rho' = 1$, $\rho = 0$, and $\eta' = \eta$. Then both Equations (4) and (16) yield

$$\begin{aligned} \psi_R &= P_0 \psi_B + \theta_B (2P_1 - P_0) \\ &+ \frac{h}{\eta} S_A P_1 + \frac{h}{2\eta} \left(S_x + \frac{S_y}{2} \right) (3P_2 - 2P_1) \end{aligned} \quad (21)$$

Also of this case both Equations (4) and (17) reduce to

$$\begin{aligned} \psi_A &= 2P_1 \psi_B + 2\theta_B (P_2 - P_1) \\ &+ \frac{S_A P_2 h}{\eta} + \frac{S_x h}{\eta} (P_3 - P_2) + \frac{S_y h}{2\eta} (P_3 - P_2) \end{aligned} \quad (22)$$

For this flow direction, it has been shown that the equations for θ_R reduce to one another to order ε^2 for $\tan^{-1}(\frac{\eta}{\mu}) = \frac{\pi}{3}$. They do not reduce to one another exactly since both are approximations.

One can obtain a unique value for the scalar flux by summing the expression for the vertex angular flux, Equation (20), over all discrete-directions. Since six triangles meet at a point, six triangles will contribute to this sum. Knowing these vertex scalar fluxes, any source, for example a fission source, which depends on the scalar flux can be computed for every vertex in the problem. If one further assumes that the source is represented by a linear expansion in each triangle then the expansion is uniquely determined by the vertex sources S_1 , S_2 , and S_3 . The leading term in this expansion is

$$(S_1 + S_2 + S_3)/3$$

If the values of the vertex sources are positive then this expansion is positive everywhere in the triangle. The leading term of the moment expansion of the source is S_A . If we multiply the unique linear expansion by the positive quantity

$$3S_A / (S_1 + S_2 + S_3) \quad ,$$

then we obtain an expansion with leading term S_A which is positive everywhere in the triangle. This expansion will have the same form as the moment expansion if we make the identifications

$$S_x \cong \frac{3(S_2 - S_1) S_A}{(S_1 + S_2 + S_3)} \quad (23)$$

and

$$S_y \cong \frac{S_A (2S_3 - S_1 - S_2)}{(S_1 + S_2 + S_3)} \quad (24)$$

Notice that if

$$S_A = (S_1 + S_2 + S_3)/3$$

we obtain the usual form for the x and y derivatives of S. If all triangles have positive inflow representations then all vertex values of the angular flux will be positive. If all angular vertex fluxes are positive then the scalar flux constructed from these angular fluxes will be positive. Hence, the vertex values of the source will be positive and the source expansion using relations 23 and 24 will be positive.

TEST PROBLEM RESULTS AND CONCLUSIONS

Two test problems were analyzed using both the DITRI scheme as implemented in the code THREETRAN (hex,z)⁶ and the TLC scheme as implemented in the code TWOHEX which is under development at the present time at Los Alamos. The first problem is a simple one energy group problem. The domain is the hexagon shown in Figure 2. The cross sections are also indicated in this figure.

The graph in Figure 4 indicates the manner in which the eigenvalue converges as the size of the triangles in the mesh is reduced. The height of a triangle in the mesh starts at 6 cm and is reduced as indicated. From the graph it is quite clear that the TLC scheme is far superior to the DITRI scheme in terms of accuracy. Table 1 under Figure 4 indicates that the TLC results are converged while the DITRI eigenvalue has not yet converged. Of course, this is a severe high leakage test problem and is simply used to test the methods. The problem is not meant to be characteristic of a reactor core.

Notice that these schemes do not converge to the same result for this problem. This is due to the fact that the THREETRAN (hex,z) code and the TWOHEX code use different quadrature sets. The THREETRAN (hex,z) code uses the 90° rotationally invariant set used by TWOTRAN-II code⁸. The TWOHEX code uses a 60 degree rotationally invariant Tschebyschev-Legendre set first described by Carlson⁹ and used in the DIAMANT2 code.⁵ The DITRI result is obtained using the S6 quadrature with 24 directions total. The TLC result is obtained by using a rectangular S4 set (2 points on each z-direction cosine level). This S4 set also has 24 directions. Additional results indicate that these two sets are converging to the same result as the number of discrete directions is increased.

The second test problem has been used before to test numerical schemes. The geometric configuration for this problem is shown in Figure 3. Region I is a highly scattering region with a source density of unity and surrounds the almost "black" central region II. The mesh for Figure 5 is 20 triangles long by 10 triangles high. In region II the side of a triangle is 5 mean free paths. The results indicate that the TLC method is much more positive than the DITRI method. No fixup of any kind is used in either of the schemes. The negative fluxes appearing in the TLC plot are so small that they are not apparent in the graph. This plot is along triangle band number 5. This problem was analyzed using the same quadrature set as in the first problem.

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Figure 1. Triangle Coordinate Systems.

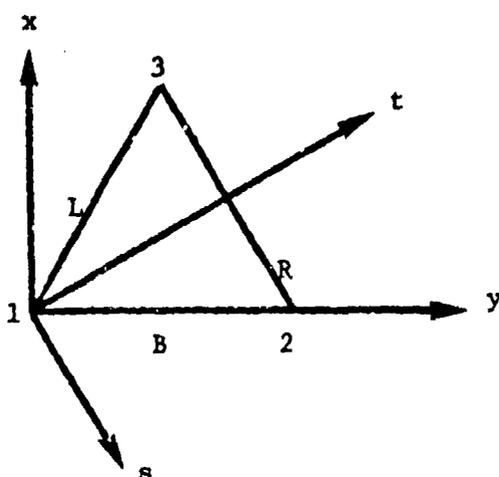
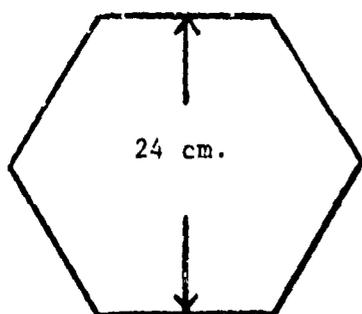
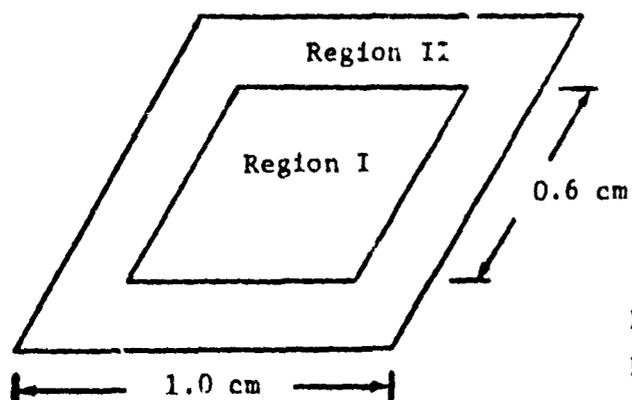


Figure 2. Problem #1.



Σ_a	$\nu\Sigma_f$	Σ_T	Σ_S
0.1	0.03	0.15	0.14

Figure 3. Problem #2.



	S	Σ_a	Σ_t	Σ_S
Region I:	0.0	100.0	100.0	0.0
Region II:	1.0	0.05	1.0	0.95

Figure 4. Eigenvalue as a function of mesh size.

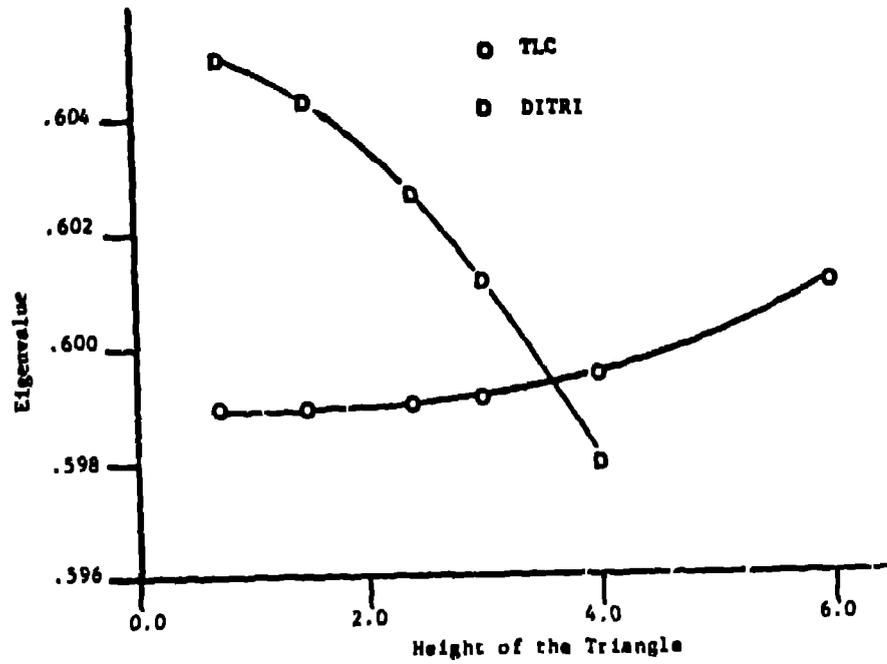


Table 1. Eigenvalue Comparison

Mesh Size (Height of Triangle) cm	Eigenvalue ^a DITRI S6	Eigenvalue ^a TLC S4 Rectangular
12.00	0.53983	0.62363
6.00	0.58919	0.60111
4.50	0.59796	0.59950
3.00	0.60115	0.59912
2.40	0.60265	0.59900
1.50	0.60424	0.59891
0.75	0.60501	0.59890

^a Converged to an error of 10^{-5}

Figure 5. Cell average scalar flux as a function of position.

