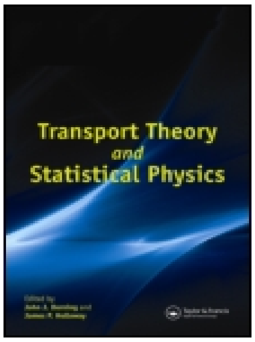

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Infinite-Medium Solutions of the Transport Equation, S_N Discretization Schemes, and the Diffusion Approximation

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ABSTRACT

In the beginning of this article, we construct a family of infinite-medium solutions of the linear transport equation. This family consists of angular fluxes that (*i*) vary linearly (or quadratically) in space and angle and (*ii*) are driven by isotropic sources that vary linearly (or quadratically) in space. Each angular flux in this family satisfies Fick's Law; thus, the corresponding scalar flux satisfies the familiar diffusion equation. Then, we show that (*i*) only certain discretization schemes for the transport equation preserve the "linear" infinite-medium solutions, and (*ii*) these schemes are more accurate in diffusive problems. More precisely, we show that the "quadratic" solutions of these discrete schemes are much more accurate for

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problems in which the cell width is not optically thin. The overall goal of this article is to demonstrate why it is advantageous for discretization schemes to preserve the ‘‘linear’’ (as well as the ‘‘flat’’) infinite-medium solutions of the transport equation.

1. INTRODUCTION

In developing discretization methods for the transport equation, several considerations help one to assess the accuracy and robustness of a proposed scheme (Alcouffe et al., 1979; Lewis and Miller, 1984). Does the scheme satisfy particle balance? Does it preserve the ‘‘infinite-medium’’ (flat isotropic source, flat isotropic angular flux) solution? In 1-D, is the scheme at least second-order accurate? If the source is positive, is the resulting angular flux guaranteed to be positive? Is the scheme robust for coarse spatial grids? Does the scheme satisfy the ‘‘diffusion limit’’ (Larsen, 1992; Larsen et al., 1987)? These last questions are theoretically difficult, particularly for multidimensional problems with unstructured spatial grids (Adams, 2001; Adams et al., 1998; Wareing, 1999). In this article, an expanded version of a recent ANS abstract (Larsen, 2001a) and conference talk (Larsen, 2001b), we develop a new theoretical technique to address these and other questions.

The new technique employs a family of low-order polynomial infinite-medium solutions of the transport equation. This family of solutions consists of angular fluxes, which are (*i*) linear (or quadratic) in space and angle, and (*ii*) driven by sources which themselves are linear (or quadratic) in space. Because of the structure of these angular fluxes they satisfy Fick’s Law, even though they are not always linear in angle. Thus, for each angular flux in this family, the corresponding scalar flux satisfies the conventional diffusion equation.

Now, we ask: how well does a given transport discretization scheme reproduce these analytic solutions? All credible transport discretization schemes (*i*) preserve the ‘‘flat’’ (flat isotropic source, flat isotropic flux) solution for all space-angle grids, and (*ii*) produce any exact solution in the fine-mesh limit. However, not all discretization schemes preserve the ‘‘linear’’ solutions on all grids. What are the consequences if a discretization scheme does (or does not) preserve ‘‘linear’’ solutions for all grids?

The purpose of this article is to explore and partly answer this question. In planar geometry, we show that among the class of Weighted Diamond discretizations of the standard discrete-ordinates (S_N) equations, only the conventional Diamond Difference scheme preserves the ‘‘linear’’ solutions for all space-angle grids. The Weighted

Diamond "linear" solutions possess a truncation error in the cell-edge angular flux. This produces a truncation error in Fick's Law, which in turn produces a truncation error in the discrete "quadratic" solution. Diamond Difference solutions do not possess this error. Thus, the failure of Weighted Diamond schemes to preserve "linear" infinite-medium solutions is directly associated with a significant loss of accuracy in diffusive problems.

This shows that it is advantageous for a transport differencing scheme to preserve the "linear" transport solutions for all space-angle grids (since then, an accurate discrete form of Fick's law holds in problems for which the angular flux is nearly linear in angle). A second benefit is that in curviliner geometries, unphysical "flux dips" at $r = 0$ are suppressed. A third likely benefit is that the numerical solution will be, overall, more grid-independent. These properties allow the computational solution to be more accurate, particularly in diffusive problems with weak spatial and angular dependence.

The work in this article directly relates to "characteristic" methods that are presently employed in S_N reactor lattice physics codes (Hong and Cho, 1998; Knott et al., 1995). A typical such method is the "Step Characteristic" scheme, in which the scattering source is approximated as a spatial histogram and the S_N equations are solved analytically along characteristic lines passing through the system in discrete-ordinates directions (Alcouffe et al., 1979). This method has several attractive features: the solution is positive and the representation of the scattering source requires minimal storage; in planar geometry the solution is second-order accurate, and is exact in a pure absorber with a histogram interior source. The Diamond-Difference solution requires the same storage and in 1-D is second-order accurate, but is not always positive and is not exact in a pure absorber. Also, the Diamond Difference solution can exhibit unphysical spatial oscillations in absorbing regions unless the spatial grid is optically thin, whereas the Step Characteristic scheme behaves monotonically.

Despite these shortcomings of the Diamond Difference scheme, we show in this article that the Diamond solution is more accurate for "diffusive" neutron transport problems. This occurs because the Step Characteristic scheme does not preserve "linear" transport solutions, and this leads to an unphysically large "effective diffusion coefficient" for spatial grids that are not optically thin.

The remainder of this article is organized as follows. In Sec. 2 we construct "linear" and "quadratic" infinite-medium solutions of the mono-energetic transport equation for 1-D planar, spherical, and cylindrical geometries. In Sec. 3 we consider Weighted Diamond planar-geometry

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S_N differencing schemes for the one-group transport equation and show that only the conventional Diamond Difference scheme preserves the "linear" solution for all space-angle grids. We also show that schemes that preserve the linear solution produce significantly more accurate "quadratic" solutions on space-angle grids that are not optically thin. In Sec. 4 we discuss related issues in spherical and cylindrical geometries. We conclude in Sec. 5 with a discussion.

2. INFINITE-MEDIUM TRANSPORT SOLUTIONS

Our analysis applies to the monoenergetic 3-D transport equation:

$$\underline{\Omega} \cdot \underline{\nabla}\psi(\underline{r}, \underline{\Omega}) + \Sigma_t \psi(\underline{r}, \underline{\Omega}) = \int_{4\pi} \Sigma_s(\underline{\Omega} \cdot \underline{\Omega}')\psi(\underline{r}, \underline{\Omega}')\, d\Omega' + \frac{1}{4\pi} q(\underline{r}), \tag{2.1}$$

where

$$\underline{r} = (x, y, z) = \text{spatial variable}, \tag{2.2a}$$

$$\underline{\Omega} = (\sqrt{1-\mu^2}\cos\gamma, \sqrt{1-\mu^2}\sin\gamma, \mu) = \text{angular variable}, \tag{2.2b}$$

and

$$\Sigma_s(\mu_0) = \sum_{k=0}^{\infty} \frac{2k+1}{4\pi} \Sigma_{sk} P_k(\mu_0)$$
$$= \text{differential scattering cross section}, \tag{2.3}$$

with $\mu_0 = \underline{\Omega} \cdot \underline{\Omega}'$ and P_k = the kth Legendre polynomial.

2.1. Planar Geometry

We first consider a planar-geometry problem with spatial variation only in the z-direction:

$$q(\underline{r}) = q(z), \tag{2.4a}$$

$$\psi(\underline{r}, \underline{\Omega}) = \psi(z, \mu). \tag{2.4b}$$

Equation (2.1) simplifies to

$$\mu \frac{\partial \psi}{\partial z}(z, \mu) + \Sigma_t \psi(z, \mu) = \int_{-1}^{1} \Sigma_s(\mu, \mu')\psi(z, \mu')\, d\mu' + \frac{q(z)}{4\pi}, \tag{2.5}$$

with

$$\Sigma_s(\mu,\mu') = \sum_{k=0}^{\infty} \frac{2k+1}{2} \Sigma_{sk} P_k(\mu) P_k(\mu'). \tag{2.6}$$

Now we construct a family of "infinite-medium" solutions of Eq. (2.5), in which the prescribed source and angular flux are both spatially quadratic:

$$q(z) = q_0 + q_1 z + q_2 z^2, \tag{2.7a}$$

$$\psi(z,\mu) = \psi_0(\mu) + \psi_1(\mu) z + \psi_2(\mu) z^2, \tag{2.7b}$$

with functions $\psi_j(\mu)$ to be determined. [Specifically, if $q(z)$ has the form of Eq. (2.7a), for any constants q_0, q_1, and q_2, we show that a solution $\psi(z,\mu)$ of Eq. (2.5) exists of the form specified by Eq. (2.7b).] Introducing Eqs. (2.7a) and Eq. (2.7b) into Eq. (2.5) and equating the coefficients of z^j, we obtain for $j = 0, 1,$ and 2

$$\Sigma_t \psi_j(\mu) - \int_{-1}^{1} \Sigma_s(\mu,\mu')\psi_j(\mu')\, d\mu' = \frac{q_j}{4\pi} - (j+1)\mu\psi_{j+1}(\mu), \tag{2.8}$$

with $\psi_3(\mu) = 0$. These equations can be solved recursively, first for $j = 2$, then $j = 1$, and then $j = 0$.

The $j = 2$ solution is isotropic:

$$\psi_2(\mu) = \frac{q_2}{4\pi\Sigma_{a0}}. \tag{2.9}$$

(We employ the notation

$$\Sigma_{an} \equiv \Sigma_t - \Sigma_{sn}, \quad n = 0, 1, 2, \tag{2.10}$$

so $\Sigma_{a0} = \Sigma_a =$ absorption cross section and $\Sigma_{a1} = \Sigma_{tr} =$ transport cross section. For now, we assume $\Sigma_{a0} \neq 0$.) The $j = 1$ solution is linear in μ:

$$\psi_1(\mu) = \frac{1}{4\pi\Sigma_{a0}}\left(q_1 - 2\mu\frac{q_2}{\Sigma_{a1}}\right), \tag{2.11}$$

and the $j = 0$ solution is quadratic in μ:

$$\psi_0(\mu) = \frac{1}{2\pi\Sigma_{a0}}\left(\frac{q_0}{2} + \frac{q_2}{3\Sigma_{a1}\Sigma_{a0}}\right) - \left(\frac{q_1}{4\pi\Sigma_{a1}\Sigma_{a0}}\right)\mu + \left(\frac{q_2}{3\pi\Sigma_{a1}\Sigma_{a2}\Sigma_{a0}}\right)P_2(\mu). \tag{2.12}$$

Introducing Eqs. (2.9), (2.11), and (2.12) into Eq. (2.7b), we obtain:

$$\psi(z,\mu) = \frac{q_0}{4\pi\Sigma_{a0}} + \left(z - \frac{\mu}{\Sigma_{a1}}\right)\frac{q_1}{4\pi\Sigma_{a0}} + \left[z^2 - \frac{2\mu z}{\Sigma_{a1}} + \frac{2}{3\Sigma_{a1}}\left(\frac{1}{\Sigma_{a0}} + \frac{3\mu^2 - 1}{\Sigma_{a2}}\right)\right]\frac{q_2}{4\pi\Sigma_{a0}}, \tag{2.13}$$

which is a second-order polynomial in z and μ. This angular flux has the following scalar flux and current:

$$\phi(z) \equiv \int_0^{2\pi}\int_{-1}^{1}\psi(z,\mu)\,d\mu\,d\gamma = \frac{1}{\Sigma_{a0}}\left[q(z) + \frac{2q_2}{3\Sigma_{a1}\Sigma_{a0}}\right], \tag{2.14a}$$

$$J(z) \equiv \int_0^{2\pi}\int_{-1}^{1}\mu\psi(z,\mu)\,d\mu\,d\gamma = -\frac{1}{3\Sigma_{a1}\Sigma_{a0}}\left[\frac{dq}{dz}(z)\right]. \tag{2.14b}$$

Thus, even though $\psi(z,\mu)$ is quadratic in μ, Fick's Law is satisfied:

$$J(z) = -\frac{1}{3\Sigma_{a1}}\frac{d\phi}{dz}(z). \tag{2.15}$$

Hence, for each quadratic angular flux $\psi(z,\mu)$ (Eq. (2.13)) driven by the source $q(z)$ (Eq. (2.7a)), the corresponding scalar flux $\phi(z)$ satisfies the standard diffusion equation:

$$-\frac{1}{3\Sigma_{a1}}\frac{d^2\phi}{dz^2}(z) + \Sigma_{a0}\phi(z) = q(z). \tag{2.16}$$

Equation (2.13) holds for $\Sigma_{a0} \neq 0$. To obtain a bounded solution for $\Sigma_{a0} = 0$, one must scale certain of the constants q_j in Eq. (2.7a) so that ψ remains bounded as $\Sigma_{a0} \to 0$. To accomplish this, we set:

$$q_1 = \Sigma_{a0}\beta_1, \tag{2.17a}$$

$$q_2 = \frac{3\Sigma_{a0}\Sigma_{a1}}{2}(\Sigma_{a0}\beta_0 - q_0), \tag{2.17b}$$

where β_0 and β_1 are arbitrary. Introducing Eq. (2.17) into Eq. (2.13), we get

$$\psi(z,\mu) = \frac{\beta_0}{4\pi} + \frac{\beta_1}{4\pi}\left(z - \frac{\mu}{\Sigma_{a1}}\right) + \frac{3\Sigma_{a1}}{4\pi}(\Sigma_{a0}\beta_0 - q_0)\left(\frac{z^2}{2} - \frac{\mu z}{\Sigma_{a1}} + \frac{3\mu^2 - 1}{3\Sigma_{a1}\Sigma_{a2}}\right). \tag{2.18}$$

Letting $\Sigma_{a0} \to 0$, we obtain:

$$q(z) = q_0, \tag{2.19}$$

$$\psi(z,\mu) = \frac{\beta_0}{4\pi} + \left(z - \frac{\mu}{\Sigma_{a1}}\right)\frac{\beta_1}{4\pi} - 3\left(\frac{\Sigma_{a1} z^2}{2} - \mu z + \frac{\mu^2 - 1/3}{\Sigma_{a2}}\right)\frac{q_0}{4\pi}. \tag{2.20}$$

In Eq. (2.20), the coefficients of β_0 and β_1 are well-known solutions of the homogeneous $\Sigma_{a0} = 0$ transport equation with no absorption (Case and Zweifel, 1967). Also, the coefficients of q_0 represent a particular solution of the $\Sigma_{a0} = 0$ transport equation with a flat isotropic source. [For $\Sigma_{a0} = 0$, no spatially linear (or quadratic) flux exists for a spatially linear (or quadratic) source. However, fluxes for such sources can be constructed that are cubic (or quartic) functions of x and μ.]

The angular flux in Eq. (2.20), for the flat source defined by Eq. (2.19), has the following scalar flux and current:

$$\phi(z) = \beta_0 + \beta_1 z - \frac{3\Sigma_{a1}}{2} q_0 z^2, \tag{2.21b}$$

$$J(z) = -\frac{\beta_1}{3\Sigma_{a1}} + q_0 z. \tag{2.28}$$

As before, these satisfy Fick's Law, and $\phi(z)$ satisfies the conventional diffusion equation with constant source q_0.

2.2. 1-D Spherical Geometry

The planar-geometry solutions derived above can be used to construct fluxes and sources with 1-D spherical symmetry. To do this, we note that if z and μ in Eqs. (2.7a) and (2.13) are replaced respectively by x and $\sqrt{1-\mu^2}\cos\gamma$, or by y and $\sqrt{1-\mu^2}\sin\gamma$, one obtains 1-D solutions of Eq. (2.1) that vary spatially in the x or y directions rather than the z-direction. Also, one can linearly combine these various fluxes and sources to obtain 3-D fluxes and sources that satisfy Eq. (2.1).

In particular, setting $q_1 = 0$ in Eq. (2.7a) and adding the sources $q(x) + q(y) + q(z)$ and the fluxes $\psi(x, \sqrt{1-\mu^2}\cos\gamma) + \psi(y, \sqrt{1-\mu^2}\sin\gamma) + \psi(z,\mu)$, we obtain the 3-D source and angular flux:

$$q(\underline{r}) = 3q_0 + (x^2 + y^2 + z^2)q_2, \tag{2.22}$$

$$\psi(\underline{r},\underline{\Omega}) = \frac{3q_0}{4\pi\Sigma_{a0}} + \left[(x^2+y^2+z^2) - \frac{2}{\Sigma_{a1}}\left(x\sqrt{1-\mu^2}\cos\gamma + y\sqrt{1-\mu^2}\cos\gamma + z\mu\right) + \frac{2}{\Sigma_{a1}\Sigma_{a0}}\right]\frac{q_2}{4\pi\Sigma_{a0}}, \tag{2.23}$$

which satisfy Eq. (2.1) and have spherical symmetry. Introducing the familiar spherical-geometry spatial and angular variables

$$r \equiv \left(x^2 + y^2 + z^2\right)^{1/2} = |\underline{r}|, \tag{2.24a}$$

$$\mu_s = \frac{x\sqrt{1-\mu^2}\cos\gamma + y\sqrt{1-\mu^2}\cos\gamma + z\mu}{(x^2+y^2+z^2)^{1/2}} = \frac{\underline{r}\cdot\Omega}{|\underline{r}|}, \tag{2.24b}$$

and replacing $3q_0$ by q_0, we obtain:

$$q(r) = q_0 + r^2 q_2, \tag{2.25}$$

$$\psi(r,\mu_s) = \frac{q_0}{4\pi\Sigma_{a0}} + \left(r^2 - \frac{2}{\Sigma_{a1}} r\mu_s + \frac{2}{\Sigma_{a1}\Sigma_{a0}}\right)\frac{q_2}{4\pi\Sigma_{a0}}. \tag{2.26}$$

The corresponding scalar flux and current are:

$$\phi(r) = \int_0^{2\pi}\int_{-1}^{1} \psi(r,\mu_s)\,d\mu_s\,d\gamma = \frac{1}{\Sigma_{a0}}\left[q(z) + \frac{2q_2}{\Sigma_{a1}\Sigma_{a0}}\right], \tag{2.27a}$$

$$J(r) = \int_0^{2\pi}\int_{-1}^{1} \mu_s\psi(r,\mu_s)\,d\mu_s\,d\gamma = -\frac{1}{3\Sigma_{a1}\Sigma_{a0}}\left[\frac{dq}{dr}(r)\right]. \tag{2.27b}$$

As before, these satisfy Fick's Law.

Equations (2.25) and (2.26) hold for $\Sigma_{a0} \neq 0$. To obtain a finite result for $\Sigma_{a0} = 0$, we scale q_2 via

$$q_2 = \frac{\Sigma_{a1}\Sigma_{a0}}{2}(\Sigma_{a0}\beta_0 - q_0)\ . \tag{2.28}$$

Then Eqs. (2.25) and (2.26) yield

$$q(r) = q_0 + \frac{\Sigma_{a1}\Sigma_{a0}}{2}(\Sigma_{a0}\beta_0 - q_0)r^2, \tag{2.29}$$

$$\psi(r,\mu_s) = \frac{\beta_0}{4\pi} + \left(r^2 - \frac{2}{\Sigma_{a1}} r\mu_s\right)\frac{\Sigma_{a1}}{8\pi}(\Sigma_{a0}\beta_0 - q_0). \tag{2.30}$$

Now letting $\Sigma_{a0} \to 0$, we obtain

$$q(r) = q_0, \tag{2.31}$$

$$\psi(r,\mu_s) = \frac{\beta_0}{4\pi} + \left(r\mu_s - \Sigma_{a1}r^2\right)\frac{q_0}{4\pi}, \tag{2.32}$$

where β_0 is arbitrary. In these equations, the coefficient of β_0 is the well-known "flat" solution of the sourceless $\Sigma_{a0} = 0$ transport equation. The coefficients of q_0 describe a particular solution of the $\Sigma_{a0} = 0$ spherical geometry transport equation with a spatially flat isotropic source.

The corresponding scalar flux and current are:

$$\phi(r) = \beta_0 - \frac{\Sigma_{a1} q_0}{2} r^2, \tag{2.33a}$$

$$J(r) = \frac{q_0}{3} r. \tag{2.33b}$$

Again, these satisfy Fick's Law.

2.3. 1-D Cylindrical Geometry

The planar-geometry solutions can also be used to construct sources and fluxes with 1-D cylindrical symmetry. To do this for $\Sigma_a \neq 0$, we set $q_1 = 0$ in Eqs. (2.7a) and (2.13) and add the sources $q(x, y) \equiv q(x) + q(y)$ and the fluxes $\psi(x, y, \mu, \gamma) \equiv \psi(x, \sqrt{1-\mu^2}\cos\gamma) + \psi(y, \sqrt{1-\mu^2}\sin\gamma)$ to obtain:

$$q(\underline{r}) = 2q_0 + (x^2 + y^2) q_2, \tag{2.34}$$

$$\psi(\underline{r}, \underline{\Omega}) = \frac{q_0}{2\pi\Sigma_{a0}} + \left[\frac{x^2+y^2}{2} - \frac{\sqrt{1-\mu^2}}{\Sigma_{a1}}(x\cos\gamma + y\sin\gamma) + \frac{1}{3\Sigma_{a1}}\left(\frac{2}{\Sigma_{a0}} + \frac{1-3\mu^2}{\Sigma_{a2}}\right)\right]\frac{q_2}{2\pi\Sigma_{a0}}, \tag{2.35}$$

which satisfy Eq. (2.1) and have cylindrical symmetry. Introducing the cylindrical-geometry spatial and angular variables

$$r = \sqrt{x^2 + y^2}, \tag{2.36a}$$

$$\cos\gamma_c = \sqrt{1-\mu^2}\left(\frac{x}{r}\cos\gamma + \frac{y}{r}\sin\gamma\right), \tag{2.36b}$$

(γ_c is the cylindrical azimuthal angle), and replacing $2q_0$ by q_0, we obtain

$$q(r) = q_0 + r^2 q_2, \tag{2.37}$$

$$\psi(r, \mu, \gamma_c) = \frac{q_0}{2\pi\Sigma_{a0}} + \left[\frac{r^2}{2} - \frac{r\cos\gamma_c}{\Sigma_{a1}} + \frac{1}{3\Sigma_{a1}}\left(\frac{2}{\Sigma_{a0}} + \frac{1-3\mu^2}{\Sigma_{a2}}\right)\right]\frac{q_2}{2\pi\Sigma_{a0}}. \tag{2.38}$$

The corresponding scalar flux and current are:

$$\phi(r) = \int_0^{2\pi}\int_{-1}^{1} \psi(r,\mu,\gamma_c)\,d\mu\,d\gamma = \frac{1}{\Sigma_{a0}}\left[q(r) + \frac{4q_2}{3\Sigma_{a1}\Sigma_{a0}}\right], \tag{2.39a}$$

$$J(r) = \int_0^{2\pi}\int_{-1}^{1} (\cos\gamma_c)\psi(r,\mu,\gamma_c)\,d\mu\,d\gamma = -\frac{1}{3\Sigma_{a1}\Sigma_{a0}}\left[\frac{dq}{dr}(r)\right], \tag{2.39b}$$

which satisfy Fick's law.

These results hold for $\Sigma_{a0} \neq 0$. To obtain a finite result for $\Sigma_{a0} = 0$, we scale q_2 via

$$q_2 = \frac{3\Sigma_{a1}\Sigma_{a0}}{4}(\Sigma_{a0}\beta_0 - q_0). \tag{2.40}$$

Then, Eqs. (2.37) and (2.38) yield

$$q(r) = q_0 + \frac{3\Sigma_{a0}\Sigma_{a1}}{4}(\Sigma_{a0}\beta_0 - q_0)r^2, \tag{2.41}$$

$$\psi(r,\mu,\gamma_c) = \frac{\beta_0}{4\pi} - \frac{3\Sigma_{a1}}{2}\left(\frac{r^2}{2} - \frac{r\cos\gamma_c}{\Sigma_{a1}} + \frac{1-\mu^2}{3\Sigma_{a1}\Sigma_{a2}}\right)\frac{q_0}{4\pi}. \tag{2.42}$$

Letting $\Sigma_{a0} \to 0$, we obtain

$$q(r) = q_0, \tag{2.43}$$

$$\psi(r,\mu,\gamma_c) = \frac{\beta_0}{4\pi} - \frac{3\Sigma_{a1}}{2}\left(\frac{r^2}{2} - \frac{r\cos\gamma_c}{\Sigma_{a1}} + \frac{1-\mu^2}{3\Sigma_{a1}\Sigma_{a2}}\right)\frac{q_0}{4\pi}, \tag{2.44}$$

where β_0 is arbitrary. The corresponding scalar flux and current are:

$$\phi(r) = \beta_0 - \frac{3\Sigma_{a1}q_0}{4}r^2, \tag{2.45a}$$

$$J(r) = \frac{q_0}{2}r. \tag{2.45b}$$

Again, these satisfy Fick's law.

3. PLANAR GEOMETRY S_N DISCRETIZATION SCHEMES

Now we examine discrete-ordinates (S_N) in angle, Weighted Diamond in space discretizations of the planar geometry transport equation [Eq. (2.5)]. A thorough discussion of these familiar discretization methods is given in (Lewis and Miller, 1984). We employ common notation and utilize a standard Gauss-Legendre quadrature set $\{\mu_n, w_n\}$ for $1 \leq n \leq N$, with N the *order* of the quadrature set. For simplicity, we assume isotropic scattering, $\Sigma_t = 1$, $\Sigma_s = c$, a spatial grid with cell edges $z_{j+1/2}$, and uniform cell width $h = z_{j+1/2} - z_{j-1/2}$.

Integrating the S_N approximation to Eq. (2.5) over the jth spatial cell $z_{j+1/2} \leq z \leq z_{j+1/2}$ and using the conventional notation for the cell-edge and cell-average fluxes (Lewis and Miller, 1984), we obtain the balance equation

$$\frac{\mu_n}{h}\left(\psi_{n,j+1/2} - \psi_{n,j-1/2}\right) + \psi_{n,j} = \frac{c}{2}\sum_{m=1}^{N} \psi_{m,j} w_m + \frac{Q_j}{2}, \tag{3.1}$$

with

$$Q_j \equiv \frac{1}{h}\int_{z_{j-1/2}}^{z_{j+1/2}} q(z)\, dz = q_0 + q_1 z_j + q_2\left(z_j^2 + \frac{h^2}{12}\right). \tag{3.2}$$

To Eq. (3.1), we append the "Weighted Diamond" (WD) auxiliary equations

$$\psi_{n,j} = \left(\frac{1+\alpha_n}{2}\right)\psi_{n,j+1/2} + \left(\frac{1-\alpha_n}{2}\right)\psi_{n,j-1/2}, \tag{3.3}$$

where α_n are the angular weights. These satisfy the constraints:

$$0 \leq \mu_n \alpha_n \leq |\mu_n| \quad \text{(stability)}, \tag{3.4a}$$

$$\mu_n = -\mu_m \quad \Rightarrow \quad \alpha_n = -\alpha_m \quad \text{(symmetry)}, \tag{3.4b}$$

but otherwise are arbitrary. The Diamond Difference (DD) scheme results from specifying $\alpha_n = 0$. The Step Characteristic (SC) scheme results from specifying (Alcouffe et al., 1979):

$$\alpha_n = \alpha_n(h) = \frac{1 + e^{-h/\mu_n}}{1 - e^{-h/\mu_n}} - \frac{2\mu_n}{h}. \tag{3.5}$$

Equations (3.1)–(3.4b) possess an exact solution with the same quadratic spatial behavior as the source. Thus, the cell-average and cell-edge fluxes have the form

$$\psi_{n,j} = f_{0,n} + f_{1,n} z_j + f_{2,n}\left(z_j^2 + \frac{h^2}{12}\right), \tag{3.6a}$$

$$\psi_{n,j+1/2} = g_{0,n} + g_{1,n} z_{j+1/2} + g_{2,n} z_{j+1/2}^2, \tag{3.6b}$$

where z_j is the center of the jth cell and the angle-dependent coefficients $f_{k,n}$ and $g_{k,n}$ are to be determined. If the discrete solution were to "preserve" the analytic solutions given by Eqs. (2.7b) and (2.13), then $f_{k,n} = g_{k,n} = \psi_k(\mu_n)$ for $0 \le k \le 2$ and $1 \le n \le N$. Unfortunately, we show that this is generally not the case.

Introducing Eq. (3.6) into Eq. (3.1), using $z_{j\pm1/2} = z_j \pm h/2$, and equating the coefficients of z_j^k for $k = 0, 1,$ and 2, we obtain six algebraic equations for $f_{k,n}$ and $g_{k,n}$. These equations can be solved, first for $f_{2,n}$ and $g_{2,n}$, then for $f_{1,n}$ and $g_{1,n}$, and then for $f_{0,n}$ and $g_{0,n}$. Omitting the algebraic details, we obtain:

$$f_{2,n} = \frac{q_2}{2(1-c)}, \tag{3.7a}$$

$$f_{1,n} = \frac{q_1}{2(1-c)} - \frac{q_2}{1-c}\mu_n, \tag{3.7b}$$

$$\begin{aligned} f_{0,n} = {} & \frac{q_0}{2(1-c)} - \frac{q_1}{2(1-c)}\mu_n + \frac{q_2}{1-c}\left[\frac{c}{3(1-c)} + \mu_n^2\right] \\ & + \frac{q_2 h}{2(1-c)}\left[\frac{\rho c}{2(1-c)} + \mu_n \alpha_n\right], \end{aligned} \tag{3.7c}$$

where

$$\rho \equiv \frac{1}{2}\sum_{n=1}^{N} \mu_n \alpha_n w_n. \tag{3.8}$$

Also,

$$g_{2,n} = f_{2,n}, \tag{3.9a}$$

$$g_{1,n} = f_{1,n} - h\alpha_n g_{2,n}, \tag{3.9b}$$

$$g_{0,n} = f_{0,n} - \frac{h}{2}\alpha_n g_{1,n} + \frac{h^2}{3} g_{2,n}. \tag{3.9c}$$

Introducing these results into Eqs. (3.6), we obtain the cell-average scalar fluxes

$$\begin{aligned}\phi_j &\equiv \sum_{n=1}^{N} \psi_{n,j} w_n \\ &= \frac{q_0}{1-c} + \frac{q_1}{1-c} z_j + \frac{q_2}{1-c}\left[\left(z_j^2 + \frac{h^2}{12}\right) + \frac{1}{1-c}\left(\frac{2}{3} + h\rho\right)\right], \qquad (3.10)\end{aligned}$$

and the cell-edge currents

$$J_{j+1/2} \equiv \sum_{n=1}^{N} \mu_n \psi_{n,j} w_n = -\frac{1}{1-c}\left(q_1 + 2q_2 z_{j+1/2}\right)\left(\frac{1}{3} + \frac{h\rho}{2}\right).$$

These quantities (automatically) satisfy the balance equation

$$\frac{1}{h}\left(J_{j+1/2} - J_{j-1/2}\right) + (1-c)\phi_j = Q_j. \qquad (3.11)$$

By inspection, they also exactly satisfy the following discrete form of Fick's Law:

$$J_{j+1/2} = -\left(\frac{1}{3} + \frac{h\rho}{2}\right)\left(\frac{\phi_{j+1} - \phi_j}{h}\right). \qquad (3.12)$$

We now discuss these results.

1. In the limit $h \to 0$,
$$f_{k,n} = \psi_k(\mu_n) = g_{k,n}, \quad 0 \le k \le 2, \quad 1 \le n \le N, \qquad (3.13)$$
where $\psi_k(\mu)$ is the coefficient of z^k in Eqs. (2.7b) and (2.13). Thus, the analytic solution is obtained in the fine (spatial) mesh limit.
2. For a constant source ($q_1 = q_2 = 0$), $f_{k,n} = \psi_k(\mu_n) = g_{k,n}$. Thus, as is well-known, all WD schemes preserve the infinite-medium "flat" solution.
3. For a linear source ($q_2 = 0$), one has for $k = 0$ and 1:
$$\begin{aligned} f_{k,n} &= \psi_k(\mu_n), \\ g_{k,n} &= \psi_k(\mu_n) - (1-k)\frac{h}{2}\alpha_n f_{1,n}. \qquad (3.14)\end{aligned}$$
Thus, the cell-average fluxes are preserved, but the cell-edge fluxes are preserved only if $\alpha_n = 0$. The only scheme under consideration

that preserves the "linear" infinite medium solution is the DD scheme, for which $\alpha_n = 0$.

4. For a quadratic source ($q_2 \neq 0$), no WD scheme preserves the complete angular flux. However, the DD solution preserves the correct cell-average scalar fluxes and cell-edge currents. (No other WD scheme does this.)
5. All discrete quadratic solutions constructed above satisfy the balance Eq. (3.11) and the Fick's Law (3.12). Equation (3.12) contains the effective diffusion coefficient:

$$D(h) = \frac{1}{3} + \frac{h\rho(h)}{2}. \tag{3.15}$$

The only considered scheme that has the correct grid-independent value of $D = 1/3$ is the Diamond scheme, for which $\rho(h) = 0$.

Previously, we showed that all analytic "quadratic" transport solutions satisfy the standard diffusion equation [Eq. (2.16)]. Using Eq. (3.12) to eliminate the currents from Eq. (3.11), we find that all the above discrete "quadratic" solutions satisfy the discrete diffusion equation

$$-\left(\frac{1}{3} + \frac{h\rho}{2}\right)\left(\frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2}\right) + (1-c)\phi_j = Q_j. \tag{3.16}$$

This discrete equation contains two types of truncation errors:

1. The error associated with the finite-difference approximation

$$\frac{d^2\phi}{dx^2} \approx \frac{\phi_{j+1} - 2\phi_j + \phi_{j-1}}{h^2},$$

which is a natural manifestation of the discretization process.

2. The error associated with the effective diffusion coefficient $D(h)$ [Eq. (3.15)].

The second error occurs for all WD differencing schemes, for which $\rho > 0$. This error is a numerical artifact that unphysically increases the flow of neutrons away from regions with high flux, into regions with low flux. Thus, it unphysically "overdiffuses," or "flattens" the solution. It has the potential to cause significant errors in the numerical estimates of the scalar flux for spatial grids in which h is not small.

To show this we plot, in Fig. 1, D vs. h for the S_2 DD and SC schemes. For $h = 1.0$ mean free path, the SC diffusion coefficient is

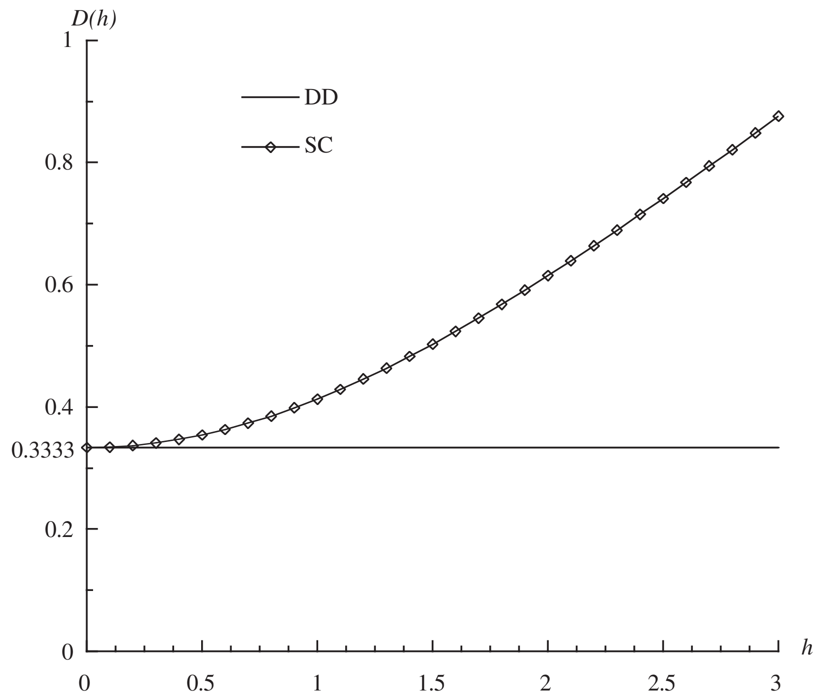

Figure 1. DD and SC diffusion coefficients.

$D = 0.4128$, representing a 24% relative error. For $h = 2.0$, the SC diffusion coefficient is $D = 0.6147$, an 86% relative error. For large h, the error in the SC $D(h)$ grows nearly linearly with h.

In Fig. 2 we plot scalar fluxes for the following problem: a 20 mean free path thick slab, $c = 1$, reflecting left boundary, vacuum right boundary, driven by a constant source with magnitude chosen so that the exact S_2 scalar flux equals unity at $z = 0$. The S_2 scalar fluxes are plotted, as are the DD and SC cell-average scalar fluxes, for $h = 1.0$ and 2.0 mean free paths.

For this problem, the DD scalar fluxes are extremely accurate, for both $h = 1.0$ and 2.0. However for these values of h, the SC scalar fluxes are inaccurate. For $h = 1.0$, the SC cell average scalar flux in the innermost cell is 0.8177, about an 18% error. For $h = 2.0$, the same flux is 0.5567, about a 44% error. The diffusion version of the given problem, solved with a diffusion coefficient that is 24% (86%) too large, yields a scalar flux that is low by the multiplicative factor $1/1.24 \approx .81$ ($1/1.86 \approx 0.54$). These estimates agree closely with the numerical results. (They do not perfectly agree because of the finite boundary at $z = 20.0$.)

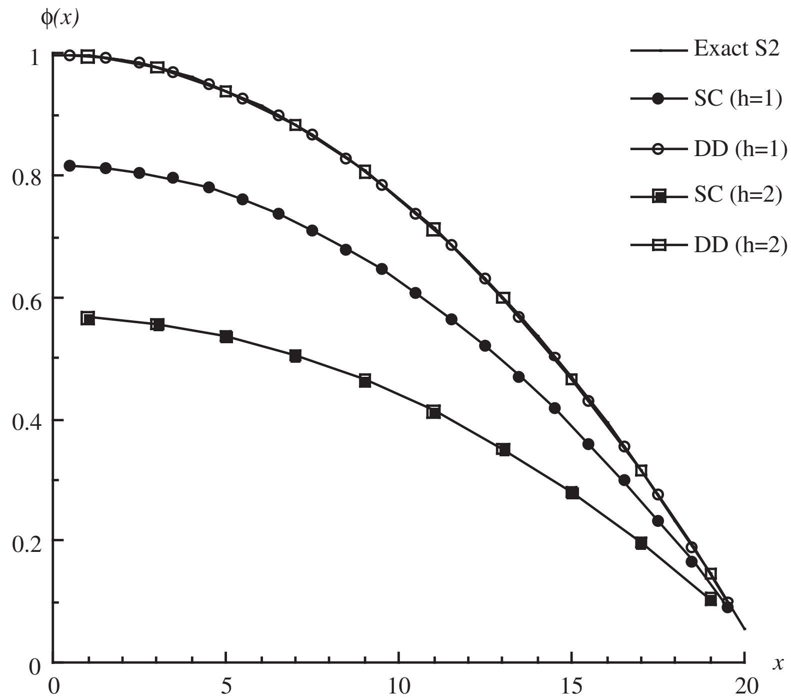

Figure 2. Exact and approximate S_2 scalar fluxes.

These calculations show that among the class of discretization schemes under consideration, the one scheme that preserves ‘‘linear’’ transport solutions—the DD scheme—is the most accurate in diffusive problems where the physical angular flux behaves, locally in space, nearly linearly in space and angle. The preceding analysis explains why this happens: WD schemes, which do not preserve the linear solution, have an unphysically large diffusion coefficient. This incorrectly ‘‘overdiffuses,’’ or ‘‘overflattens’’ the correct (fine-mesh) transport solution.

There may be another use of the quadratic infinite medium solutions constructed in Sec. 2. These ‘‘quadratic’’ angular fluxes all have scalar fluxes that satisfy the conventional diffusion equation. Thus, for finite-medium problems, if one solves the conventional diffusion equation—with boundary conditions that are perfectly consistent with the exact quadratic angular flux—one obtains the exact scalar flux and current. However, it is easily shown that conventional Marshak, Mark, or other known boundary conditions are not consistent with an angularly quadratic angular flux! Thus, although the diffusion equation is capable of yielding the exact scalar fluxes, conventional boundary conditions do not permit this to happen. By modifying the diffusion boundary conditions, it might be possible to robustly preserve the quadratic scalar fluxes generated in this article, thereby yielding improvements in accuracy for more general problems. This idea will not be pursued further here.

4. SPHERICAL AND CYLINDRICAL GEOMETRY S_N SCHEMES

We now briefly discuss two subjects relevant to transport discretization schemes in 1-D spherical and cylindrical geometries.

First, the spherical geometry transport equation contains an angular derivative that must be discretized. Originally, the "Diamond" angular differencing scheme

$$\psi_{n,j} = \frac{1}{2}\left(\psi_{n+1/2,j} + \psi_{n-1/2,j}\right) \tag{4.1}$$

was used in spherical geometry S_N codes. However, Morel proposed a "Weighted Diamond" angular differencing scheme

$$\psi_{n,j} = \frac{1+\beta_n}{2}\psi_{n+1/2,j} + \frac{1-\beta_n}{2}\psi_{n-1/2,j}, \tag{4.2}$$

in which the weights β_n are uniquely chosen so that the angular flux can vary linearly in angle (Morel and Montry, 1984) [Eq. (4.1) does not permit ψ to vary linearly in angle, because angular quadrature points μ_n do not generally lie midway between $\mu_{n-1/2}$ and $\mu_{n+1/2}$.]. Morel's scheme does allow ψ to vary linearly in angle. This scheme significantly improves the accuracy of the resulting calculations, greatly suppressing the infamous "flux dip" at $r = 0$. In terms of the analysis in the present article, we would say that Morel's modification enables the spherical geometry S_N equations to preserve the quadratic-in-space, linear-in-angle solutions given by Eqs. (2.25) and (2.26) (for $c < 1$), and Eqs. (2.31) and (2.32) (for $c = 1$). The "Diamond" angular differencing scheme [Eq. (4.1)] does not preserve these spherically-symmetric solutions.

Also, because the spherical geometry, quadratic-in-space, linear-in-angle solutions are actually linear in angle—not quadratic, as in planar geometry—simple diffusion boundary conditions, such as the Marshak condition, will exactly preserve these solutions when used with the conventional diffusion equation. Thus, there may exist a simplicity in the spherical geometry diffusion boundary condition that is lacking in planar geometry!

In 1-D cylindrical geometry, Morel's "Weighted Diamond in angle" approach again enables solutions that vary linearly in $\underline{\Omega}$ to be preserved. Interestingly, the 1-D cylindrical solutions in Eq. (2.38) are not linear in angle, as the corresponding solutions are in spherical geometry. It is not clear whether exact cylindrical-geometry solutions can be constructed that depend linearly on $\underline{\Omega}$. Nonetheless, calculations show that Morel's approach does significantly suppress angular truncation errors in 1-D cylindrical geometry S_N problems.

5. DISCUSSION

We have constructed a family of infinite-medium solutions of the monoenergetic transport equation, consisting of angular fluxes that are (*i*) linear (or quadratic) in space and angle, and (*ii*) driven by sources that are linear (or quadratic) in space. These angular fluxes satisfy Fick's law; therefore, their scalar fluxes satisfy the conventional diffusion equation.

We also investigated a class of transport discretization schemes and showed that a scheme that preserves the "linear" infinite medium solutions has a more accurate discrete form of Fick's law, and this yields more accurate solutions for diffusive problems. (Other benefits of preserving the linear solution are that numerical solutions are less dependent on the spatial grid, and in curvilinear geometries, unphysical "flux dips" at $r = 0$ are suppressed.) For these reasons, it is advantageous for transport discretization schemes to preserve the "flat" and "linear" infinite medium solutions.

Requiring a discretization scheme to preserve the "linear" infinite-medium transport solutions is more difficult than requiring the scheme to preserve only the flat infinite-medium transport solutions. Even so, this is less difficult than requiring a scheme to preserve the exact solution in the absence of scattering—which certain characteristic methods are able to fulfill in planar geometry but not in other geometries (Knott et al., 1995; Hong and Cho, 1998).

The analysis in this article is relevant to the accuracy of transport discretization schemes applied to "diffusive" problems. An earlier asymptotic analysis has addressed similar concerns (Larsen, 1992). The asymptotic and the present analyses are complementry in several ways:

1. It is relatively easy to determine whether an S_N spatial differencing scheme preserves the linear solution on a structured or

unstructured grid. However, the asymptotic analysis can be difficult to implement, particularly for multidimensional problems with unstructured grids (Adams, 2001; Adams et al., 1998; Wareing et al., 1999).

2. The asymptotic analysis has been developed mainly for radiative transfer problems in which spatial cells are optically thick. A different but related asymptotic analysis has been developed for neutron transport problems with spatial cells that are on the order of one mean free path in thickness, but this approach has received much less attention (Larsen, 1983). The method developed in the present article is (*i*) distinct from both of these asymptotic analyses, and (*ii*) applicable to all spatial grids, regardless of whether the grid is optically thin, thick, structured, or unstructured.

We conjecture that a *necessary* condition for a transport discretization scheme to be accurate and robust in diffusive problems is that it preserves the linear transport solutions. Unfortunately, this condition is *not sufficient* for problems with optically thick spatial cells. (The DD preserves the linear solution, but instabilities interfere with the robustness of this scheme in optically thick grids.) However, the ‘‘linearity’’ condition might be necessary and sufficient for common neutron transport schemes with spatial cells on the order of one mean free path in thickness. This question will not be pursued here.

In his article, we have focused our attention on monoenergetic transport problems. However, the same analysis can clearly be applied to energy-dependent problems. If an infinite-medium energy-dependent source with a polynomial dependence in space is prescribed, it will drive an infinite-medium energy-dependent angular flux, which has the ‘‘same’’ polynomial dependence in angle and space (The energy dependence of the source and angular flux will generally not be polynomial.) It is possible that new information could be gained by comparing fully-discrete (in space, angle, and energy) solutions to exact continuous (in space, angle, and energy) of the transport equation. However, this question too will not be pursued here.

Finally, we comment that in the development of discretization methods for the diffusion equation, considerable importance has been placed on the ability of a (diffusion) discretization scheme to preserve spatially ‘‘linear’’ solutions (Kershaw, 1981; Morel et al., 1992; Morel et al., 1998; Palmer, 2001). Experience and theory indicate that when solutions are preserved, numerical solutions of more general diffusion problems are more accurate and robust. In this article, we suggest that a similar principle applies to the transport equation. The main extra complication with the transport equation is that "linear" solutions vary linearly in both space *and* angle.

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