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TITLE: **ASYMPTOTIC DERIVATION OF THE SIMPLIFIED P_n EQUATIONS**

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ASYMPTOTIC DERIVATION OF THE SIMPLIFIED P_N EQUATIONS

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ABSTRACT

The diffusion and simplified P_N equations are derived from the transport equation by means of an asymptotic expansion in which the diffusion equation is the leading order approximation and the simplified P_N equations are higher-order approximations. In addition, the simplified P_N equations are reformulated in a "canonical" form that greatly facilitates the formulation of boundary conditions and the implementation of the resulting problem in a conventional multigroup diffusion code. Numerical comparisons of S_N, diffusion, and simplified P_N solutions show that the simplified P_N solutions often contain most of the transport corrections for the diffusion approximation.

I. INTRODUCTION

The spherical harmonic or P_N equations have been a well-known and widely-used approximation to the transport equation for the past 50 years. This approximation has the following properties:

1. The angularly-dependent transport equation is replaced by a finite system of equations in which the angular variable is explicitly absent.

2. As the order N of the approximation increases, one recovers the exact transport solution.

3. The P_N equations are rotationally invariant; their solutions are free of ray effects.

4. In three-dimensional geometry, the number of P_N equations equals N^2. In planar geometry, the number of P_N equations is only N.

5. For $N > 1$, the P_N equations are not known to have a positive solution.

To deal with the large number and complexity of the P_N equations, Gelbard[1-3,10] and other researchers[4-9,11-15] have proposed a "simplified P_N" (SP_N) approximation in which the number of equations equals N (hence is significantly less than with the multidimensional P_N equations), but one abandons the requirement that the exact transport solution is obtained as $N \to \infty$. Instead, the goal is to obtain a relatively inexpensive generalization of diffusion theory that contains most of the transport physics lacking in diffusion theory. Presently, the SP_N equations have an incomplete theoretical foundation. Nevertheless, they have been tested in 1-D as well as 2-D and 3-D problems, and the reported numerical results are impressive. For many problems, low-order SP_N equations capture most (Gamino[13] reports "greater than 80%") of the transport corrections to the diffusion approximation.

In this paper, we show that the SP_N equations are robust high-order asymptotic approximations of the transport equation in a physical regime in which the conventional P_1 equations are the leading-order approximation. In other words, SP_N theories contain higher-order asymptotic corrections to P_1 theory. This explains the high accuracy often exhibited by numerical solutions of the SP_N equations.

We also reformulate the SP_3 equations in a new "canonical" form. For planar-geometry problems, this form reduces to the second-order even-parity S_N equations, and for general isotropic scattering problems, it reduces to a conventional system having the form of multigroup diffusion equations. Because of these properties, the canonical form (*i*) makes the question of boundary conditions for these equations almost trivial, (*ii*) greatly facilitates the implementation of the SP_3 problem in a standard multigroup diffusion code, and (*iii*) shows that for a proper choice of boundary conditions, the solutions of the SP_3 equations are positive. This canonical form can be obtained for any odd-order system of SP_N equations.

Finally, we present multidimensional numerical results obtained from a test code utilizing the canonical form of the SP_N equations. As earlier work has shown, we find that low-order SP_N solutions are a significant improvement over P_1 solutions and are obtained at a small fraction of the cost of an S_N calculation.

The remainder of this paper is organized as follows. In Section II we asymptotically derive the P_1, SP_2, and SP_3 equations for the one-group transport equation with isotropic scattering. (Higher-order SP_N equations can be derived by continuing this procedure.) In Section III, we reformulate the SP_3 equations into "canonical" form, and we propose boundary conditions for this new form. In Section IV we present numerical results. We conclude in Section V with a discussion.

II. ASYMPTOTIC ANALYSIS

In this paper we shall consider the one-group three-dimensional transport equation with isotropic scattering:

$$\underline{\Omega} \cdot \nabla\psi(\underline{r},\underline{\Omega}) + \Sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega}) = \frac{\Sigma_s(\underline{r})}{4\pi}\int \psi(\underline{r},\underline{\Omega}')d\Omega' + \frac{Q(\underline{r})}{4\pi} \quad . \tag{1}$$

More complex (multigroup, anisotropic scattering) problems require a more complicated asymptotic analysis that we will present elsewhere. We consider Eq. (1) under the scaling:

$$\Sigma_t(\underline{r}) = \frac{\sigma_t(\underline{r})}{\varepsilon} \quad , \tag{2}$$

$$\Sigma_a(\underline{r}) = \varepsilon\sigma_a(\underline{r}) \quad , \tag{3}$$

$$\Sigma_s(\underline{r}) = \Sigma_t(\underline{r}) - \Sigma_a(\underline{r}) = \frac{\sigma_t(\underline{r})}{\varepsilon} - \varepsilon\sigma_a(\underline{r}) \quad , \tag{4}$$

$$Q(\underline{r}) = \varepsilon q(\underline{r}) \quad , \tag{5}$$

where σ_t, σ_a, and q are $O(1)$ and $\varepsilon \ll 1$. The physics implied by this scaling is:

1. The system is optically thick ($\Sigma_t \gg 1$).

2. The rates of absorption and production due to interior sources are comparable and weak [$\Sigma_a = O(\varepsilon)$ and $Q = O(\varepsilon)$].
3. The infinite medium solution $\phi = Q/\Sigma_a = q/\sigma_a$ is $O(1)$.
4. The diffusion length $L = (3\Sigma_t\Sigma_a)^{-1/2} = (3\sigma_t\sigma_a)^{-1/2}$ is $O(1)$.
5. If one introduces the scaling defined by Eqs. (2)-(5) into the standard diffusion approximation to Eq. (1), the resulting equation is independent of ε. In other words, the standard diffusion equation is invariant under the scaling (2)-(5).

The scaling defined by Eqs. (2)-(5) has long been known[16,17] to be one in which transport theory asymptotically transitions into diffusion theory as $\varepsilon \to 0$. In this paper, we show that higher-order asymptotic corrections to diffusion theory yield simplified P_N theories.

To begin, we introduce Eqs. (2)-(5) into Eq. (1) and multiply by ε/σ_t to get

$$\left(I + \frac{\varepsilon}{\sigma_t}\underline{\Omega}\cdot\underline{\nabla}\right)\psi = \frac{1}{4\pi}\left[\left(1 - \varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2\frac{q}{\sigma_t}\right] \quad , \tag{6}$$

where

$$\phi(\underline{r}) = \int \psi(\underline{r}, \underline{\Omega}')d\Omega' \quad . \tag{7}$$

Next, we invert the operator on the left side of Eq. (6) and integrate over $\underline{\Omega}$ to obtain the Peierls integral equation for the scalar flux:

$$\phi = \left[\frac{1}{4\pi}\int\left(I + \frac{\varepsilon}{\sigma_t}\underline{\Omega}\cdot\underline{\nabla}\right)^{-1}d\Omega\right]\left[\left(1 - \varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2\frac{q}{\sigma_t}\right] \quad . \tag{8}$$

If there are non-vacuum boundary conditions, then extra terms occur in Eq. (8). However, these are $O(e^{-\rho/\varepsilon})$, where ρ is the optical distance to the boundary. Thus, in the interior of the system these terms are exponentially small and we will ignore them.

Next, we formally expand the operator on the right side of Eq. (8) in powers of ε. We obtain

$$\phi = \left(\sum_{n=0}^{\infty}\varepsilon^{2n}\mathcal{L}_{2n}\right)\left[\left(1 - \varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2\frac{q}{\sigma_t}\right] \quad , \tag{9}$$

where

$$\mathcal{L}_{2n} = \frac{1}{4\pi}\int\left(\frac{1}{\sigma_t}\underline{\Omega}\cdot\underline{\nabla}\right)^{2n}d\Omega \quad . \tag{10}$$

The operators $\mathcal{L}_0$, $\mathcal{L}_2$, and $\mathcal{L}_4$ are explicitly defined by

$$\mathcal{L}_0 = I \quad , \tag{11}$$

$$\mathcal{L}_2 = \frac{1}{3}\sum_{i,j=1}^{3}(\delta_{ij})\left(\frac{1}{\sigma_t}\frac{\partial}{\partial x_i}\frac{1}{\sigma_t}\frac{\partial}{\partial x_j}\right) = \frac{1}{\sigma_t}\underline{\nabla}\cdot\frac{1}{3\sigma_t}\underline{\nabla} \quad , \tag{12}$$

$$\mathcal{L}_4 = \frac{1}{15}\sum_{i,j,k,l=1}^{3}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\left(\frac{1}{\sigma_t}\frac{\partial}{\partial x_i}\frac{1}{\sigma_t}\frac{\partial}{\partial x_j}\frac{1}{\sigma_t}\frac{\partial}{\partial x_k}\frac{1}{\sigma_t}\frac{\partial}{\partial x_l}\right) \quad . \tag{13}$$

If the system is homogeneous or the problem has spatial variation in only one direction, the formulas for $\mathcal{L}_{2n}$, $n \geq 2$, simplify to:

$$\mathcal{L}_{2n} = \frac{3^n}{2n+1}(\mathcal{L}_2)^n \quad . \tag{14}$$

In our analysis, we shall replace the original definition of $\mathcal{L}_{2n}$ [Eq. (10)] by Eq. (14). This is rigorously correct for a homogeneous system or for a spatially one-dimensional problem, but not for a true multidimensional problem at material interfaces. We shall discuss this approximation again in Sec. V.

Introducing Eq. (14) into Eq. (9), we get

$$\phi = \left(I + \varepsilon^2 \mathcal{L}_2 + \frac{9\varepsilon^4}{5}\mathcal{L}_2^2 + \frac{27\varepsilon^6}{7}\mathcal{L}_2^3 + O\left(\varepsilon^8\right)\right)\left[\left(1 - \varepsilon^2 \frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2 \frac{q}{\sigma_t}\right] \quad . \tag{15}$$

Formally inverting the operator on the right side of this equation, we obtain:

$$\left(I - \varepsilon^2 \mathcal{L}_2 - \frac{4\varepsilon^4}{5}\mathcal{L}_2^2 - \frac{44\varepsilon^6}{35}\mathcal{L}_2^3 + O\left(\varepsilon^8\right)\right)\phi = \left(1 - \varepsilon^2 \frac{\sigma_a}{\sigma_t}\right)\phi + \varepsilon^2 \frac{q}{\sigma_t} \quad , \tag{16}$$

or

$$-\sigma_t \left(\mathcal{L}_2\phi + \frac{4\varepsilon^2}{5}\mathcal{L}_2^2\phi + \frac{44\varepsilon^4}{35}\mathcal{L}_2^3\phi + O\left(\varepsilon^6\right)\right) + \sigma_a\phi = q \quad . \tag{17}$$

If we now retain terms of $O(\varepsilon^{2n})$ but discard all higher order terms, we obtain a partial differential equation for ϕ of order $2n$. This equation is an asymptotic approximation to the Peierls equation (8), but it is not any of the simplified P_N approximations. To derive these approximations, we must rewrite the equation obtained from Eq. (17) in an asymptotically equivalent form as either a single second-order equation or as a coupled system of second-order equations. We shall now give the details of this procedure.

II.1 Diffusion (P_1) Equation

We delete terms of $O(\varepsilon^2)$ and higher in Eq. (17) and use the definition (12) to get

$$-\underline{\nabla} \cdot \frac{1}{3\sigma_t}\underline{\nabla}\phi + \sigma_a\phi = q \quad . \tag{18}$$

Multiplying this equation by ε and using the definitions (2)-(5), we obtain

$$-\underline{\nabla} \cdot \frac{1}{3\Sigma_t(\underline{r})}\underline{\nabla}\phi(\underline{r}) + \Sigma_a(\underline{r})\phi(\underline{r}) = Q(\underline{r}) \quad . \tag{19}$$

This is the conventional diffusion (P_1) equation.

II.2 Simplified P_2 Equation

We delete terms of $O(\varepsilon^4)$ and higher in Eq. (17) and rearrange slightly to get

$$\left(I + \frac{4\varepsilon^2}{5}\mathcal{L}_2\right)\mathcal{L}_2\phi = \frac{\sigma_a\phi - q}{\sigma_t} \quad . \tag{20}$$

Operating on this equation by $(I - 4\varepsilon^2\mathcal{L}_2/5)$ and again deleting terms of $O(\varepsilon^4)$, we obtain

$$\mathcal{L}_2\phi = \left(I - \frac{4\varepsilon^2}{5}\mathcal{L}_2\right)\frac{\sigma_a\phi - q}{\sigma_t} \quad , \tag{21}$$

or, using Eq. (12),

$$-\underline{\nabla} \cdot \frac{1}{3\sigma_t}\underline{\nabla}\left(\phi + \frac{4\varepsilon^2}{5}\frac{\sigma_a\phi - q}{\sigma_t}\right) + \sigma_a\phi = q \quad . \tag{22}$$

Multiplying this equation by ε and using the definitions (2)-(5), we obtain

$$-\underline{\nabla}\cdot\frac{1}{3\Sigma_t(\underline{r})}\underline{\nabla}\left(\phi(\underline{r})+\frac{4}{5}\frac{\Sigma_a(\underline{r})\phi(\underline{r})-Q(\underline{r})}{\Sigma_t(\underline{r})}\right)+\Sigma_a(\underline{r})\phi(\underline{r})=Q(\underline{r}) \quad . \tag{23}$$

This is the SP_2 equation.

II.3 Simplified P_3 Equations

Now we delete terms of $O(\varepsilon^6)$ in Eq. (17) to obtain

$$-\sigma_t\mathcal{L}_2\left(\phi+\frac{4\varepsilon^2}{5}\mathcal{L}_2\phi+\frac{44\varepsilon^4}{35}\mathcal{L}_2^2\phi\right)+\sigma_a\phi=q \quad . \tag{24}$$

Hence, if we define

$$\xi(\underline{r})=\frac{2\varepsilon^2}{5}\mathcal{L}_2\phi(\underline{r})+\frac{22\varepsilon^4}{35}\mathcal{L}_2^2\phi(\underline{r})=\left(I+\frac{11\varepsilon^2}{7}\mathcal{L}_2\right)\frac{2\varepsilon^2}{5}\mathcal{L}_2\phi(\underline{r}) \quad , \tag{25}$$

then Eq. (24) can be written

$$-\sigma_t\mathcal{L}_2(\phi+2\xi)+\sigma_a\phi=q \quad . \tag{26}$$

Operating on Eq. (25) by $(I-11\varepsilon^2\mathcal{L}_2/7)$ and again deleting terms of $O(\varepsilon^6)$, we get

$$\left(-\frac{11\varepsilon^2}{7}\mathcal{L}_2+I\right)\xi=\frac{2\varepsilon^2}{5}\mathcal{L}_2\phi \quad . \tag{27}$$

Now, multiplying Eq. (26) by ε and using the definitions (2)-(5) and (12), we obtain

$$-\underline{\nabla}\cdot\frac{1}{3\Sigma_t(\underline{r})}\underline{\nabla}[\phi(\underline{r})+2\xi(\underline{r})]+\Sigma_a(\underline{r})\phi(\underline{r})=Q(\underline{r}) \quad . \tag{28}$$

Likewise, multiplying Eq. (27) by σ_t/ε and using the definitions (2)-(5) and (12), we obtain

$$-\underline{\nabla}\cdot\frac{1}{3\Sigma_t(\underline{r})}\underline{\nabla}\left[\frac{11}{7}\xi(\underline{r})+\frac{2}{5}\phi(\underline{r})\right]+\Sigma_t(\underline{r})\xi(\underline{r})=0 \quad . \tag{29}$$

Eqs. (28) and (29) are the SP_3 equations.

We note that the three-dimensional P_1, SP_2, and SP_3 results derived above could have been obtained by the following ad-hoc procedure:

1. Write the planar-geometry P_N approximations to Eq. (1) in second order form (i.e., eliminate the odd angular flux moments).
2. Replace the one-dimensional diffusion operator by its three-dimensional generalization:

$$\left(\frac{d}{dx}\frac{1}{\Sigma_t}\frac{d}{dx}\right)\rightarrow\left(\underline{\nabla}\cdot\frac{1}{\Sigma_t}\underline{\nabla}\right) \quad . \tag{30}$$

This, in fact, is the procedure that has previously been used to derive the SP_N equations. The asymptotic analysis presented above, which can easily be extended to higher-order SP_N approximations, legitimizes the results of this procedure by showing that for certain problems, the SP_N equations are an asymptotic approximation to the transport equation. The problems for which this is *strictly* true are ones for which Eq. (14) holds for $n\geq 2$, i.e.,

1. Multidimensional problems in a medium in which Σ_t is constant (but Σ_s can vary).

2. One-dimensional problems in an inhomogeneous medium.

The problems for which this is *approximately* true are:

1. Truly diffusive problems, in which $\mathcal{L}_{2n}\phi \approx 0$ for $n \geq 2$. (For these problems, the higher-order asymptotic corrections are negligible, so the approximations made in deriving them play no role.)

2. Multidimensional problems in inhomogeneous media for which the solution at interfaces is locally one-dimensional in the direction normal to the interface.

Thus, for multidimensional heterogeneous nondiffusive problems, the SP_N equations for $n \geq 2$ are not strict asymptotic approximations to the transport equation. However, they are very closely related to asymptotic approximations, and numerical calculations show that in many problems, they contain most of the transport physics that is lacking in the P_1 approximation.

III. CANONICAL FORM OF THE SP_3 EQUATIONS

We now rewrite Eqs. (28) and (29) in "canonical" form. To do this, we multiply Eq. (29) by a constant λ and add the result to Eq. (28). This yields

$$-\underline{\nabla}\cdot\frac{1}{\Sigma_t}\underline{\nabla}\left[\frac{\phi+2\xi}{3}+\lambda\left(\frac{2\phi}{15}+\frac{11\xi}{21}\right)\right]+\Sigma_t(\phi+\lambda\xi)=\Sigma_s\phi+Q \quad . \tag{31}$$

Now we seek constants μ^2 and λ such that for arbitrary functions $\phi(\underline{r})$ and $\xi(\underline{r})$,

$$\frac{\phi+2\xi}{3}+\lambda\left(\frac{2\phi}{15}+\frac{11\xi}{21}\right)=\mu^2(\phi+\lambda\xi) \quad . \tag{32}$$

We easily obtain two solutions; for $n = 1$ and 2,

$$\mu_n^2=\frac{15+(-1)^n 2\sqrt{30}}{35} \quad : \quad \mu_1\approx 0.340 \quad , \quad \mu_2\approx 0.861 \quad , \tag{33}$$

$$\lambda_n=\frac{5}{2}\left(3\mu_n^2-1\right) \quad : \quad \lambda_1\approx -1.633 \quad , \quad \lambda_2\approx 3.061 \quad . \tag{34}$$

Hence, if we define

$$\psi_n(\underline{r})=\phi(\underline{r})+\lambda_n\xi(\underline{r}) \quad , \quad n=1,2 \quad , \tag{35}$$

then Eqs. (31) and (32) imply

$$-\underline{\nabla}\cdot\frac{\mu_n^2}{\Sigma_t}\underline{\nabla}\psi_n+\Sigma_t\psi_n=\Sigma_s\phi+Q \quad , \quad n=1,2 \quad . \tag{36}$$

Also, if we define

$$w_1=\frac{\lambda_2}{\lambda_2-\lambda_1}\approx 0.652 \quad , \quad w_2=\frac{\lambda_1}{\lambda_1-\lambda_2}\approx 0.348 \quad , \tag{37}$$

then

$$\phi(\underline{r})=\psi_1(\underline{r})w_1+\psi_2(\underline{r})w_2 \quad , \tag{38}$$

and Eqs. (36) can be written

$$-\underline{\nabla}\cdot\frac{\mu_n^2}{\Sigma_t(\underline{r})}\underline{\nabla}\psi_n(\underline{r})+\Sigma_t(\underline{r})\psi_n(\underline{r})=\Sigma_s(\underline{r})\sum_{m=1}^{2}\psi_m(\underline{r})w_m+Q(\underline{r}) \quad , \quad n=1,2 \quad . \tag{39}$$

This is the "canonical" form of the SP_3 equations. The constants μ_n, w_n in these equations constitute the usual planar-geometry S_4 Gauss-Legendre quadrature set. Therefore, in planar geometry, the canonical SP_3 equations reduce to the even-parity S_4 equations. In general geometry, the canonical SP_3 equations (with isotropic scattering) take the form of two-group diffusion equations with upscattering.

Eqs. (39) could have been obtained from Eq. (1) by the following ad-hoc procedure:

1. Write the planar-geometry even-parity S_4 approximation to Eq. (1) using the S_4 Gauss-Legendre quadrature set:

$$-\frac{d}{dx}\frac{\mu_n^2}{\Sigma_t}\frac{d}{dx}\psi_n+\Sigma_t\psi_n=\Sigma_s\sum_{m=1}^{2}\psi_m w_m+Q \quad , \quad n=1,2 \quad . \tag{40}$$

2. Make the same operator replacement as shown in Eq. (30), i.e.,

$$\left(\frac{d}{dx}\frac{1}{\Sigma_t}\frac{d}{dx}\right)\rightarrow\left(\underline{\nabla}\cdot\frac{1}{\Sigma_t}\underline{\nabla}\right) \quad . \tag{41}$$

Eqs. (39) are algebraically equivalent to the the SP_N equations for the following reason. The planar geometry even-parity S_4 equations (40) are algebraically equivalent to the planar geometry P_3 equations. Thus, introducing the operator replacement (41) in Eqs. (40), we obtain Eqs. (39), and introducing the same operator replacement in the planar geometry P_3 equations, we obtain Eqs. (28) and (29).

We now turn to the question of boundary conditions for Eqs. (39). In principle, one could derive SP_3 boundary conditions using a high-order asymptotic boundary layer analysis, but this leads to a very complex result that is difficult to implement. Instead, we shall invoke the following "one-dimensional" principle: because Eqs. (39) reduce to the even-parity S_4 equations (40) for planar geometry problems, the boundary conditions for Eqs. (39) should reduce to the standard even-parity S_4 boundary conditions for planar geometry problems. For multidimensional problems in which the solutions have a locally one-dimensional character near the boundary, this principle seems reasonable and intuitive.

Thus, for $\underline{r}$ a point on the outer boundary with $\underline{n}$ the unit outer normal, reflecting boundary conditions that satisfy the one-dimensional principle are

$$\underline{n}\cdot\underline{\nabla}\psi_n(\underline{r})=0 \quad , \quad n=1,2 \quad . \tag{42}$$

Also, for $\underline{r}$ a boundary point at which an incident flux $f(\underline{r},\underline{\Omega})$ is prescribed for $\underline{\Omega}\cdot\underline{n}<0$, boundary conditions that satisfy the one-dimensional principle are

$$f_n(\underline{r})=\psi_n(\underline{r})+\frac{\mu_n}{\Sigma_t(\underline{r})}\underline{n}\cdot\underline{\nabla}\psi_n(\underline{r}) \quad , \quad n=1,2 \quad . \tag{43}$$

Here we have defined

$$f_1(\underline{r})=\frac{1}{\mu_1 w_1}\int_{0<-\underline{\Omega}\cdot\underline{n}<w_1}|\underline{\Omega}\cdot\underline{n}|\,f(\underline{r},\underline{\Omega})d\Omega \quad , \tag{44}$$

$$f_2(\underline{r}) = \frac{1}{\mu_2 w_2} \int_{w_1 < -\Omega \cdot \underline{n} < 1} |\Omega \cdot \underline{n}| \, f(\underline{r}, \Omega) d\Omega \quad . \tag{45}$$

We note that f_1 and f_2 are proportional to the incoming partial currents over the angular "cones" that correspond to μ_1 and μ_2. The definition of these functions ensures that

$$\sum_{n=1}^{2} \mu_n f_n(\underline{r}) w_n = \int_{\Omega \cdot \underline{n} < 0} |\Omega \cdot \underline{n}| \, f(\underline{r}, \Omega) d\Omega \quad . \tag{46}$$

Therefore, for one-dimensional and multidimensional problems that behave in a locally one-dimensional manner near the outer boundary, the total incoming partial current is preserved.

We have shown that the canonical SP_3 equations are useful for prescribing boundary conditions. However, these equations have other important advantages:

1. They can easily be implemented in a conventional multigroup diffusion code.
2. Because solutions of standard multigroup diffusion problems are guaranteed to be positive, this is also true for solutions of multigroup diffusion SP_3 problems. This guarantee does not exist for solutions of standard SP_3 problems (with boundary conditions that are not equivalent to those given above) or of conventional P_3 problems.
3. The SP_3 equations are tightly coupled and often require acceleration for efficient solution. However, the canonical SP_3 equations, which so closely resemble the even-parity S_4 equations, can easily make use of diffusion acceleration procedures that apply to the even-parity S_4 equations[18]. Lack of space prevents a full discussion of this here.

The procedure described above can easily be applied to higher order SP_N appproximations. For example, the canonical SP_5 equations take the form of a three-group diffusion problem with boundary conditions that are patterned after Eqs. (42)-(45). For planar geometry, these equations reduce to the conventional even-parity S_6 equations.

IV. NUMERICAL RESULTS

First we shall consider two 3-D k-eigenvalue test problems for which the conventional diffusion solutions are inaccurate. These problems utilize a 3-D 2-group model of a small light-water reactor containing a core, a reflector and a control rod. They are described as Model 1, Case 1 (control rod out) and Model 1, Case 2 (control rod in) in the benchmark problems compiled by Takeda and Ikeda[19]. We solved these problems using the NIKE code[20,21], with a uniform 1.0 cm^3 mesh, on the CM2 computer at Los Alamos National Laboratory. The diffusion, canonical SP_N, and S_4 eigenvalues and running times are plotted in Figure 1.

We see that for both problems, the low-order canonical SP_N calculations require significantly less computational time than the S_4 calculations. Also, the low-order SP_N results for the "rod in" problem are significantly more accurate than the diffusion results. The SP_N results for the "rod out" problem are more accurate than the diffusion results, but are less accurate than the "rod in" problem results. This is because the "rod out" problem contains a region with long neutron streaming paths. Hence, this problem contains transport effects that are not well-described by any diffusion or SP_N approximation.

Next, we consider a 3-D problem in which classic ray effects are observed in S_N solutions. This problem consists of a homogeneous, one-group, isotropically scattering 130 cm cube with $\sigma_t = 0.05$

cm^{-1}, σ_s = 0.0025 cm^{-1} (c=0.05), six vacuum boundaries, and a uniform isotropic source in a 17.3 cm sub-cube situated in one corner. The system is depicted in Figure 2. In Figure 3, various S_N and canonical SP_N scalar fluxes are plotted along the line $x = 26$ cm, $z = 43.3$ cm, and $0 \leq y \leq 80$ cm. These results were also calculated with NIKE. Figure 3 shows that the S_N solutions all contain ray effects, which tend to diminish as N increases. However, the SP_1 (diffusion) and SP_3 solutions contain no ray effects, the diffusion solution is inaccurate, and the SP_3 solution agrees basically with the S_{16} solution. (The SP_5 solution, which is not shown in the figure, agrees very closely with the SP_3 solution.)

We conclude that although SP_N solutions do not limit to the exact transport solution as $N \to \infty$, they also do not contain the ray effect errors that are inherent in the S_N equations, which *do* limit to the exact transport equation as $N \to \infty$.

V. DISCUSSION

In this paper, we have derived the conventional and canonical SP_N equations from the transport equation using a high-order asymptotic expansion in which the diffusion equation is the leading-order approximation and the SP_N equations are higher-order approximations.

Problems in which the SP_N equations are not accurate contain significant multidimensional heterogeneities that generate strong multidimensional space and angular variations in the angular flux. Problems in which the SP_N equations are accurate are ones in which the multidimensional spatial and angular variations are weak, or if strong spatial and angular variations occur, they are locally one-dimensional in nature. This is depicted in Figure 4.

In summary, we have shown that the excellent numerical SP_N results obtained by previous researchers is not accidental. The SP_N equations are often just as theoretically valid an approximation of the transport equation as the P_1 equations, and as a practical matter, they are usually much more accurate. They should be useful in many problems for which conventional diffusion theory is not a sufficiently accurate approximation to transport theory.

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Figure 1: Model LWR Problems - Results

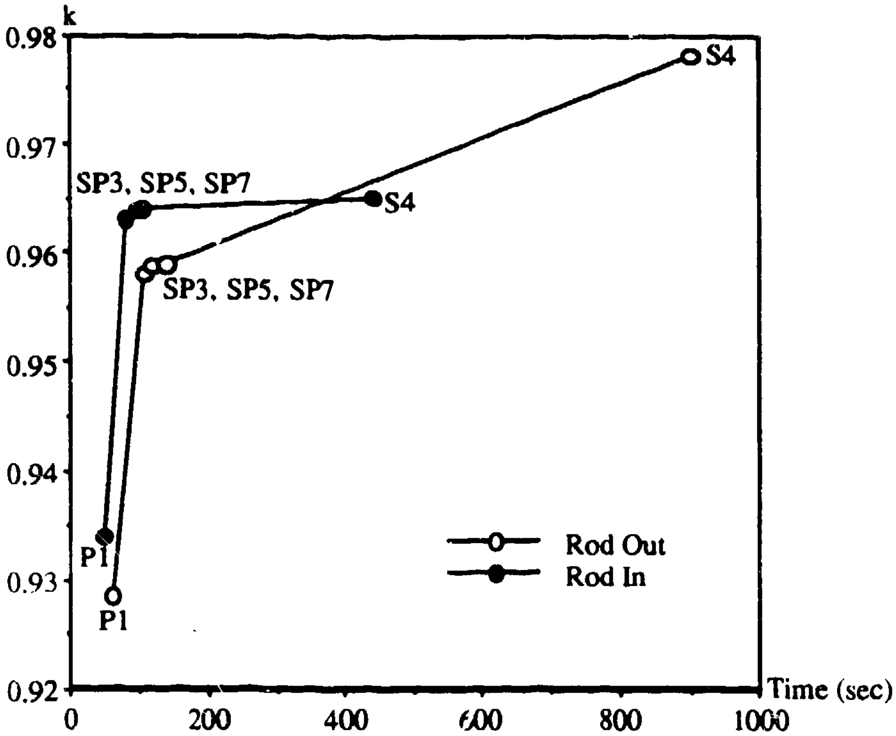

Figure 2: 3-D Ray Effect Problem (Geometry)

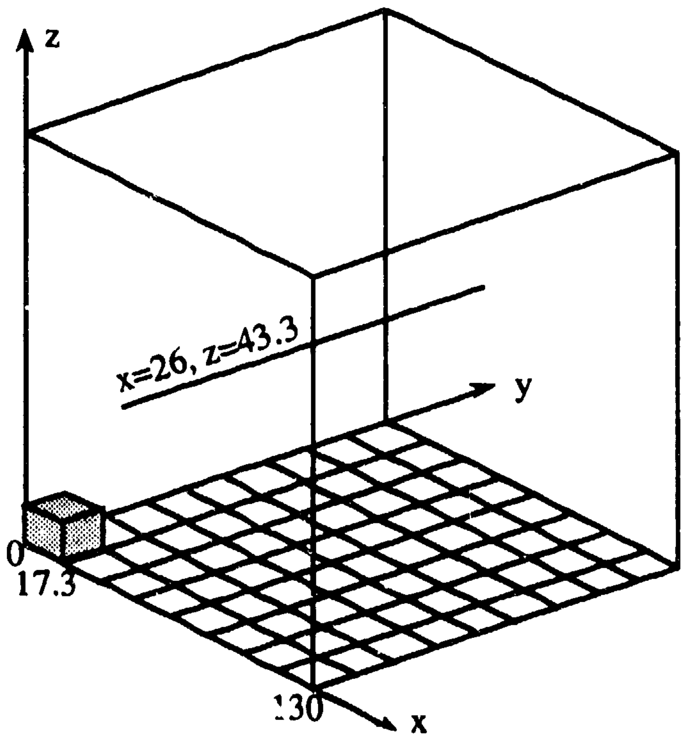

Figure 3: 3-D Ray Effect Problem (S_N and SP_N Scalar Fluxes)

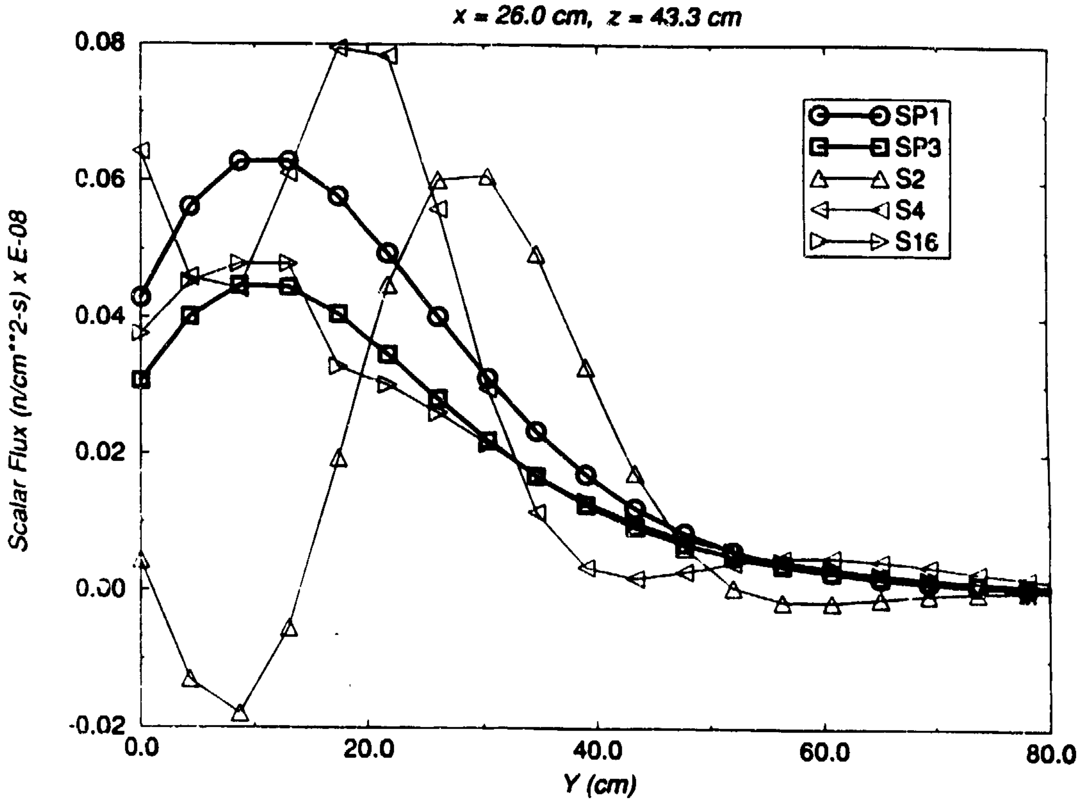

Figure 4: Qualitative Performance of Diffusion and SP_N Solutions (Each theory is valid for problems that lie to the left of its curve.)