THE NONCLASSICAL SIMPLIFIED P_2 AND P_3 EQUATIONS WITH ANISOTROPIC SCATTERING

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ABSTRACT

In classical transport, the locations of scattering centers (atoms, molecules, etc.) are not spatially correlated, and as a result, the distribution of free path lengths of particles which travel through such media is exponential. However, in certain inhomogeneous media, the locations of scattering centers *are* spatially correlated, leading to a free path length distribution that is not exponential. The theory of nonclassical transport seeks to accurately model particle transport in such nonclassical media. In this nonclassical transport theory, no assumption is made about the shape of the particle's free path length distribution, and the free path length of the particle is allowed to be an independent variable in the nonclassical transport equation. For diffusive regimes, one can approximate this equation using nonclassical versions of the simplified spherical harmonic equations (SP_N). Recently, a novel mathematical method to explicitly derive the nonclassical SP_N equations with anisotropic scattering was proposed. In this work, we use this method to explicitly derive the first three of these equations, this being the first time in which nonclassical SP_2 and SP_3 equations with anisotropic scattering are given. These equations are generalizations of previous results, and can be shown to reduce to their nonclassical counterparts with isotropic scattering and to their classical counterparts with anisotropic scattering. The nonclassical SP_N equations with anisotropic scattering are then expressed in modified forms so that vacuum boundary conditions can be applied. Finally, these modified equations are validated numerically in slab geometry, showing that they become more accurate as the system becomes more diffusive.

KEYWORDS: asymptotic analysis, nonclassical transport, anisotropic scattering, stochastic systems

1. INTRODUCTION

To successfully model particle transport through any medium, characteristics of the medium that affect particle interactions must be incorporated into the model. In traditional media, transport is *classical*, meaning that a particle performs a Brownian random walk throughout the medium because the locations of the scattering centers within the medium are not correlated with each other. This fact implies that the distribution of free path lengths taken by particles is exponential. In certain heterogeneous media, however, the locations of the scattering centers are correlated. This is most easily envisioned as a medium in which voids (or near voids) of various shapes and sizes are distributed within the medium (it can also be envisioned as a collection of material "chunks" of various shapes and sizes distributed within a void). Physical examples include pebble bed reactors, water droplets in clouds, and bubbles within a liquid. Within such media, a particle performs a Brownian random walk within the non-void material, but traverses voids with no interaction.

These flights across voids are longer on average than are expected by Brownian motion, so that the total flight (through material and void) is no longer a Brownian random walk, but is more accurately modeled as a Lèvy random walk, or Lèvy flight. Further, the free path length distribution generated from Lèvy flights has a heavy tail, and is not exponential. Particle transport with these characteristics is called *nonclassical*. Nonclassical transport occurs in many applications, including pebble-bed reactors [1], neutron transport in boiling water reators (in which the statistically longer flights take place within the bubbles) [2], in photon transport in clouds [3], in Lorentz gases [4], and in computer graphics [5]. To model nonclassical transport, the total macroscopic cross section Σ_t is assumed to be a function of the free path length s. The s-dependent steady-state, monoenergetic Boltzmann equation for the nonclassical angular flux $\hat{\psi}$ can be written as [6]

$$\begin{aligned}\frac{\partial}{\partial s}\hat{\psi}(\boldsymbol{x},\boldsymbol{\Omega},s)+\boldsymbol{\Omega}\cdot\nabla\hat{\psi}(\boldsymbol{x},\boldsymbol{\Omega},s)+\Sigma_t(s)\hat{\psi}(\boldsymbol{x},\boldsymbol{\Omega},s)& \\ =\int_{4\pi}\int_0^\infty c\Sigma_t(s')P(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\hat{\psi}(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'd\Omega'+\frac{Q(\boldsymbol{x})}{4\pi},&\end{aligned}\tag{1}$$

where a particle's position and direction are given by $\boldsymbol{x}=(x,y,z)$ and $\boldsymbol{\Omega}=(\Omega_x,\Omega_y,\Omega_z)$, respectively, with $|\boldsymbol{\Omega}|=1$, c is the scattering ratio, and Q is an isotropic interior particle source. The distribution of particles moving in direction $\boldsymbol{\Omega}'$ that scatter into direction $\boldsymbol{\Omega}$ is given by the Legendre polynomial expansion

$$P(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')=\sum_{m=0}^{\infty}\frac{2m+1}{4\pi}a_mP_m(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}'),\tag{2}$$

where P_m is the mth order Legendre polynomial with its corresponding expansion coefficient a_m, where $a_0=1$, $a_1=\bar{\mu}_0$ (the mean scattering cosine), and $\mu_0=\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}'$. The scalar flux $\Phi(\boldsymbol{x})$ can be recovered from the solution of Eq. (1) by integrating over the free-path s and angle,

$$\Phi(\boldsymbol{x})=\int_{4\pi}\int_0^\infty\hat{\psi}(\boldsymbol{x},\boldsymbol{\Omega},s)dsd\Omega.\tag{3}$$

The free path length distribution is given by

$$p(s)=\Sigma_t(s)e^{-\int_0^s\Sigma_t(s')ds'},\tag{4}$$

with its m^{th} raw moment given by

$$\langle s^m\rangle=\int_0^\infty s^m\,p(s)ds.\tag{5}$$

If transport is classical, then Eqs. (4) and (5) reduce to their classical counterparts,

$$p(s)=\Sigma_te^{-s},\quad\text{and}\quad\langle s^m\rangle=\frac{m!}{\Sigma_t^m},\tag{6}$$

respectively.

The rest of this paper is organized as follows: in Section 2 we briefly sketch the asymptotic analysis that is used to obtain a method to generate the nonclassical SP$_N$ equations with anisotropic scattering; this theory is given in detail elsewhere [7,8]. Section 3 presents the novel nonclassical SP$_2$ and SP$_3$ equations, derived explicitly here for the first time. Section 4 expresses these equations in modified forms so that vacuum boundary conditions can be applied, and Section 5 presents the numerical validation of the nonclassical SP$_N$ equations with anisotropic scattering. The paper ends in Section 6 with a discussion of the work presented.

2. SKETCH OF THE ASYMPTOTIC ANALYSIS

In this section we present only a brief sketch of the asymptotic analysis used to derive the method to generate nonclassical SP$_N$ equations with anisotropic scattering. The full analysis is given in detail in [7,8].

The scaling approach follows the one used in [9], in which $0 < \varepsilon \ll 1$. We define:

$$\Sigma_t(s) = \frac{\sigma(s/\varepsilon)}{\varepsilon},\ Q(\boldsymbol{x}) = \varepsilon q(\boldsymbol{x}),\ 1 - c = \varepsilon^2\kappa, \tag{7}$$

where κ and q are $O(1)$. This scaling leads to the scaled raw moment

$$\langle s^m \rangle = \varepsilon^m \int_0^\infty \left(\frac{s}{\varepsilon}\right)^m \frac{\sigma(s/\varepsilon)}{\varepsilon} e^{-\int_0^s \frac{\sigma(s'/\varepsilon)}{\varepsilon} ds'} ds = \varepsilon^m \langle s^m \rangle_\varepsilon, \tag{8}$$

where $\langle s^m \rangle_\varepsilon$ is O(1). For a small ε, the system is diffusive, implying that the system is optically thick and scattering dominates absorption and source strength. Applying these scaling relationships, we define Ψ such that it satisfies

$$\hat{\psi}(\boldsymbol{x}, \boldsymbol{\Omega}, \varepsilon s) \equiv \Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) \frac{e^{-\int_0^s \frac{\sigma(s'/\varepsilon)}{\varepsilon} ds'}}{\varepsilon \langle s \rangle_\varepsilon}, \tag{9}$$

where $\langle s \rangle_\varepsilon$ is the first scaled moment of s. Applying this definition and the scaling relationships to Eq. (1) results in the scaled nonclassical transport equation

$$\begin{aligned}\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) &+ \varepsilon \boldsymbol{\Omega} \cdot \nabla \int_0^s \Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s') ds' \\ &= \int_{4\pi} \int_0^\infty (1 - \varepsilon^2\kappa) p(s') P(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') \Psi(\boldsymbol{x}, \boldsymbol{\Omega}', s') ds' d\Omega' + \varepsilon^2 \langle s \rangle_\varepsilon \frac{q(\boldsymbol{x})}{4\pi}.\end{aligned} \tag{10}$$

Next, we define the following:

$$\varphi(\boldsymbol{x}, s) \equiv \int_{4\pi} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) d\Omega, \quad \text{and} \quad \Im(\cdot) \equiv \frac{1}{4\pi} \int_{4\pi} (\cdot) d\Omega, \tag{11}$$

which is an operator that averages its argument over the unit sphere. We apply the analysis described in [7,8] to write Eq. (10) as

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \frac{1}{4\pi} \sum_{i=0}^{\infty} (-1)^i \varepsilon^i \left[\mathcal{L}^{-1}(I - \Im) \boldsymbol{\Omega} \cdot \nabla \int_0^s (\cdot) ds'\right]^i \varphi(\boldsymbol{x}, s), \tag{12}$$

where the operator $\mathcal{L}^{-1}$ is

$$\mathcal{L}^{-1}\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} Y_n^m(\boldsymbol{\Omega}) L_n^{-1} \chi_n^m(\boldsymbol{x}, s), \tag{13a}$$

with

$$L_n^{-1} g(\boldsymbol{x}, s) = g(\boldsymbol{x}, s) + \frac{(1 - \varepsilon^2\kappa) b_n}{1 - (1 - \varepsilon^2\kappa) b_n} \int_0^\infty p(s') g(\boldsymbol{x}, s') ds', \tag{13b}$$

$$\chi_n^m(\boldsymbol{x}, s) = \int_{4\pi} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}', s) \bar{Y}_n^m(\boldsymbol{\Omega}') d\Omega'. \tag{13c}$$

The b_n coefficients are identical to the Legendre polynomial coefficients for $n \geq 1$; the exception is $b_0 = 0$. Equation (10) can be written as [7,8]

$$\left(\sum_{n=0}^{\infty} \varepsilon^{2n} V_n \nabla^{2n}\right) \Phi(\boldsymbol{x}) = (1 - \varepsilon^2 \kappa) \left(\sum_{n=0}^{\infty} \varepsilon^{2n} U_n \nabla^{2n}\right) \Phi(\boldsymbol{x}) + \varepsilon^2 \langle s \rangle_\varepsilon q(\boldsymbol{x}), \tag{14}$$

which can be written more compactly as

$$\left(\sum_{n=0}^{\infty} \left[W_{n+1} \nabla^{2(n+1)} + \kappa U_n \nabla^{2n}\right]\right) \Phi(\boldsymbol{x}) = \langle s \rangle_\varepsilon q(\boldsymbol{x}), \tag{15}$$

where $W_n = V_n - U_n$, and the scalar flux $\Phi(\boldsymbol{x})$ is given by

$$\Phi(\boldsymbol{x}) = \int_{4\pi} \int_0^{\infty} \Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) \frac{e^{-\int_0^s \sigma_t(s') ds'}}{\langle s \rangle_\varepsilon} ds d\Omega = \int_0^{\infty} \varphi(\boldsymbol{x}, s) \frac{e^{-\int_0^s \sigma_t(s') ds'}}{\langle s \rangle_\varepsilon} ds. \tag{16}$$

To generate the nonclassical SP$_N$ equations with anisotropic scattering, we must expand Eq. (15) to $n = N - 1$, determine the constants V_n and U_n, and rescale the equation using Eqs. (7) and (8).

3. NONCLASSICAL SP$_N$ EQUATIONS WITH ANISOTROPIC SCATTERING

The nonclassical SP$_1$ equation with anisotropic scattering, first derived in [6] using a different method, can also be derived using the asymptotic method in the previous section. It is given by

$$-\frac{1}{3}\left[\frac{\langle s^2 \rangle}{2\langle s \rangle} + \frac{c\bar{\mu}_0}{1 - c\bar{\mu}_0} \langle s \rangle\right] \nabla^2 \Phi(\boldsymbol{x}) + \frac{1 - c}{\langle s \rangle} \Phi(\boldsymbol{x}) = Q(\boldsymbol{x}), \tag{17}$$

where $\bar{\mu}_0$ is the mean scattering cosine. This result is identical to the equation derived in [6].

3.1. Derivation of the Nonclassical SP$_2$ Equation with Anisotropic Scattering

To derive the nonclassical SP$_2$ Equation with anisotropic scattering, we expand Eq. (12) to

$$\begin{aligned}\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \frac{1}{4\pi} \varphi(\boldsymbol{x}, s) - \frac{1}{4\pi} \varepsilon \left[\mathcal{L}^{-1}(I - \Im) \boldsymbol{\Omega} \cdot \nabla \int_0^s (\cdot) ds'\right] \varphi(\boldsymbol{x}, s) \\ - \frac{1}{4\pi} \varepsilon^3 \left[\mathcal{L}^{-1}(I - \Im) \boldsymbol{\Omega} \cdot \nabla \int_0^s (\cdot) ds'\right]^3 \varphi(\boldsymbol{x}, s) + O(\varepsilon^4),\end{aligned} \tag{18}$$

where each of the operators in brackets is evaluated using Eqs. (13). When completed, Eq. (18) can be written in operator form as

$$\begin{aligned}\left(I - \frac{1}{3}\varepsilon^2 \nabla^2 \int_0^s A_1(\cdot) ds - \frac{4}{45} \varepsilon^4 \nabla^4 \int_0^s A_1 A_2 A_1(\cdot) ds' + O(\varepsilon^5)\right) \varphi(\boldsymbol{x}, s) \\ = (1 - \varepsilon^2 \kappa) \int_0^{\infty} p(s) \varphi(\boldsymbol{x}, s) ds + \varepsilon^2 \langle s \rangle q(\boldsymbol{x}),\end{aligned} \tag{19}$$

where the operator A_n is defined as

$$A_n(\cdot) \equiv L_n^{-1}\left[\int_0^s (\cdot)ds\right] = \int_0^s (\cdot)ds + d_n \int_0^\infty p(s')\left(\int_0^{s'}(\cdot)ds\right)ds'. \tag{20}$$

Here, $d_n = \frac{ca_n}{1-ca_n}$, with a_n representing the n^{th} order Legendre polynomial coefficient. The right side of Eq. (19) is a function of only $\boldsymbol{x}$, implying that we can write

$$\varphi(\boldsymbol{x}, s) = g(s)\phi(\boldsymbol{x}), \tag{21}$$

where $\phi(\boldsymbol{x})$ is some unspecified function of $\boldsymbol{x}$. We can then write $g(s)$ and $\phi(\boldsymbol{x})$ in series form as

$$g(s) = g_0(s) + \varepsilon^2 g_2(s) + \varepsilon^4 g_4(s) + O(\varepsilon^5), \tag{22}$$
$$\phi(\boldsymbol{x}) = \phi_0(\boldsymbol{x}) + \varepsilon^2\phi_2(\boldsymbol{x}) + \varepsilon^4\phi_4(\boldsymbol{x}) + O(\varepsilon^5). \tag{23}$$

Additionally, we can express the integral on the right side of Eq. (19) as a series using the classical scalar flux given by Eq. (16).

After inserting Eqs. (22) and (23) into Eq. (19), discarding $O(\varepsilon^5)$ terms, and evaluating, Eq. (19) is expressed in the form of Eq. (15) as

$$\left(W_1\nabla^2 + \varepsilon^2\left[W_2\nabla^4 + \kappa U_1\nabla^2\right]\right)\Phi(\boldsymbol{x}) + \kappa\Phi(\boldsymbol{x}) = \langle s\rangle_\varepsilon q(\boldsymbol{x}). \tag{24}$$

This equation contains a fourth-order spatial derivative, and therefore is not in the desired form. To write it in a second-order derivative form (resembling the form of a diffusion equation), we write Eq. (24) as

$$-\left(I + \varepsilon^2\frac{W_2\nabla^2 + \kappa U_1}{W_1}\right)W_1\nabla^2\Phi(\boldsymbol{x}) = \kappa\Phi(\boldsymbol{x}) - \langle s\rangle_\varepsilon q(\boldsymbol{x}), \tag{25}$$

and then operate on it using $\left(I - \varepsilon^2\left[W_2\nabla^2 + \kappa U_1\right]/W_1\right)$ and discard terms of $O(\varepsilon^4)$, resulting in

$$W_1\nabla^2\left[\Phi(\boldsymbol{x}) - \varepsilon^2\frac{W_2}{W_1^2}\left[\kappa\Phi(\boldsymbol{x}) - \langle s\rangle_\varepsilon q(\boldsymbol{x})\right]\right] + \kappa\left[1 - \varepsilon^2\kappa\frac{U_1}{W_1}\right]\Phi(\boldsymbol{x}) = \left[1 - \varepsilon^2\kappa\frac{U_1}{W_1}\right]\langle s\rangle_\varepsilon q(\boldsymbol{x}), \tag{26}$$

which is now in the desired (scaled) form. The unscaled SP_2 equation is displayed in Section 3.3.

3.2. Derivation of the Nonclassical SP_3 Equation with Anisotropic Scattering

To generate the nonclassical SP_3 equation with anisotropic scattering, we expand Eq. (12) to the next odd term, resulting in

$$\begin{aligned}\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) &= \frac{1}{4\pi}\varphi(\boldsymbol{x}, s) - \frac{1}{4\pi}\varepsilon\left[\mathcal{L}^{-1}(I - \Im)\boldsymbol{\Omega}\cdot\nabla\int_0^s(\cdot)ds'\right]\varphi(\boldsymbol{x}, s)\\ &- \frac{1}{4\pi}\varepsilon^3\left[\mathcal{L}^{-1}(I - \Im)\boldsymbol{\Omega}\cdot\nabla\int_0^s(\cdot)ds'\right]^3\varphi(\boldsymbol{x}, s)\\ &- \frac{1}{4\pi}\varepsilon^5\left[\mathcal{L}^{-1}(I - \Im)\boldsymbol{\Omega}\cdot\nabla\int_0^s(\cdot)ds'\right]^5\varphi(\boldsymbol{x}, s) + O(\varepsilon^6).\end{aligned} \tag{27}$$

As in the SP_2 case, after evaluation we can write this equation in operator form as

$$\left(I - \frac{1}{3}\varepsilon^2\nabla^2 \int_0^s A_1(\cdot)ds - \frac{4}{45}\varepsilon^4\nabla^4 \int_0^s A_1A_2A_1(\cdot)ds + O(\varepsilon^5)\right)\varphi(\boldsymbol{x},s)$$
$$-\left(\frac{4}{4725}\varepsilon^6\nabla^6 \int_0^s \left(27A_1A_2A_1A_2A_1(\cdot) + 28A_1A_2A_3A_2A_1(\cdot)\right)ds + O(\varepsilon^7)\right)\varphi(\boldsymbol{x},s)$$
$$= (1-\varepsilon^2\kappa)\int_0^\infty p(s)\varphi(\boldsymbol{x},s)ds + \varepsilon^2\langle s\rangle q(\boldsymbol{x}). \tag{28}$$

The right side of Eq. (28) is a function of only $\boldsymbol{x}$. Thus, we use Eq. (21) with

$$g(s) = g_0(s) + \varepsilon^2 g_2(s) + \varepsilon^4 g_4(s) + \varepsilon^6 g_6(s) + O(\varepsilon^7), \tag{29}$$
$$\phi(\boldsymbol{x}) = \phi_0(\boldsymbol{x}) + \varepsilon^2\phi_2(\boldsymbol{x}) + \varepsilon^4\phi_4(\boldsymbol{x}) + \varepsilon^6\phi_6(\boldsymbol{x}) + O(\varepsilon^7). \tag{30}$$

Evaluating Eq. (28) with Eqs. (29) and (30) and discarding terms of $O(\varepsilon^7)$, this equation is expressed in the form of Eq. (15) as

$$\left(W_1\nabla^2 + \varepsilon^2\left[W_2\nabla^4 + \kappa U_1\nabla^2\right] + \varepsilon^4\left[W_3\nabla^6 + \kappa U_2\nabla^4\right]\right)\Phi(\boldsymbol{x}) + \kappa\Phi(\boldsymbol{x}) = \langle s\rangle_\varepsilon q(\boldsymbol{x}). \tag{31}$$

To express this equation in the form of a diffusion equation, we first define

$$\nu(\boldsymbol{x}) \equiv \left(I + \frac{\varepsilon^2}{W_2}\left[W_3\nabla^2 + \kappa U_2\right]\right)\frac{\varepsilon^2}{2}\frac{W_2}{W_1}\nabla^2\Phi(\boldsymbol{x}), \tag{32}$$

so that we can write Eq. (31) as

$$W_1\nabla^2\left[\Phi(\boldsymbol{x}) + 2\nu(\boldsymbol{x}) + \varepsilon^2\kappa\frac{U_1}{W_1}\Phi(\boldsymbol{x})\right] + \kappa\Phi(\boldsymbol{x}) = \langle s\rangle_\varepsilon Q(\boldsymbol{x}), \tag{33}$$

which is in the desired (scaled) form. We still have two unknowns and only one equation, so we operate on Eq. (32) by$(I - \varepsilon^2/W_2\left[W_3\nabla^2 + \kappa U_2\right])$ and discard terms of $O(\varepsilon^6)$ to yield

$$-\varepsilon^2 W_1\nabla^2\left[\frac{W_3}{W_1W_2}\nu(\boldsymbol{x}) + \frac{1}{2}\frac{W_2}{W_1^2}\Phi(\boldsymbol{x})\right] + \left[1 - \varepsilon^2\kappa\frac{U_2}{W_2}\right]\nu(\boldsymbol{x}) = 0. \tag{34}$$

The unscaled SP_3 equations are displayed in Section 3.3.

3.3. The Nonclassical SP_2 and SP_3 Equations with Anisotropic Scattering

Applying the scaling relationships given by Eqs. (7) and (8) to Eq. (26), the nonclassical SP_2 equation with anisotropic scattering is

$$\alpha_1\nabla^2\left[\Phi(\boldsymbol{x}) + \rho_1\left[(1-c)\Phi(\boldsymbol{x}) - \langle s\rangle Q(\boldsymbol{x})\right]\right] + \frac{1-c}{\langle s\rangle}\left[1-\gamma_1(1-c)\right]\Phi(\boldsymbol{x}) = \left[1-\gamma_1(1-c)\right]Q(\boldsymbol{x}). \tag{35}$$

Applying the scaling relationships to Eqs. (33) and (34), the nonclassical SP_3 equations with anisotropic scattering are

$$\alpha_1\nabla^2\left[\left(1+\gamma_1(1-c)\right)\Phi(\boldsymbol{x}) + 2\nu(\boldsymbol{x})\right] + \frac{1-c}{\langle s\rangle}\Phi(\boldsymbol{x}) = Q(\boldsymbol{x}), \tag{36a}$$
$$\alpha_1\nabla^2\left[\rho_2\nu(\boldsymbol{x}) + \frac{1}{2}\rho_1\Phi(\boldsymbol{x})\right] + \frac{1-\gamma_2(1-c)}{\langle s\rangle}\nu(\boldsymbol{x}) = 0, \tag{36b}$$

where $\Phi(\boldsymbol{x})$ is the scalar flux, $\nu(\boldsymbol{x})$ is the second term in a Taylor series expansion of the scalar flux, and

$$\alpha_1 = -\frac{1}{3}\frac{k_1}{\langle s\rangle}, \quad \gamma_1 = -\frac{1}{k_1}\left[k_1 - \frac{k_2}{\langle s\rangle}\right],$$

$$\rho_1 = \frac{1}{k_1^2}\left[k_{10} + \frac{4}{5}k_4\right] - \frac{1}{k_1}\frac{k_2}{\langle s\rangle}, \quad \gamma_2 = \frac{U_2}{W_2}, \quad \rho_2 = \frac{W_3}{W_1 W_2}, \quad W_1 = -\frac{1}{3}k_1,$$

$$U_2 = -\left[\frac{1}{9}k_{10} + \frac{4}{45}k_4\right] + \frac{k_9}{\langle s\rangle} + \frac{1}{9}\frac{k_2}{\langle s\rangle}\left[k_1 - \frac{k_2}{\langle s\rangle}\right],$$

$$W_2 = \frac{1}{9}k_{10} + \frac{4}{45}k_4 - \frac{1}{9}k_1\frac{k_2}{\langle s\rangle},$$

$$\begin{aligned} W_3 = &-\frac{44}{945}\left[\frac{\langle s^6\rangle}{6!} + d_1\langle s\rangle\frac{\langle s^5\rangle}{5!} + d_2 k_1\frac{\langle s^4\rangle}{4!}\right] - \frac{16}{675}\left[k_3\frac{\langle s^3\rangle}{3!} + d_2 k_4\frac{\langle s^2\rangle}{2} + d_1 k_5\langle s\rangle\right] \\ &- \frac{4}{175}\left[k_6\frac{\langle s^3\rangle}{3!} + d_2 k_7\frac{\langle s^2\rangle}{2} + d_1 k_8\langle s\rangle\right] - \frac{1}{27}\left[\frac{\langle s^6\rangle}{6!} + d_1\langle s\rangle\frac{\langle s^5\rangle}{5!} + d_1 k_2\frac{\langle s^3\rangle}{3!}\right] \\ &- \frac{4}{135}\left[\frac{\langle s^6\rangle}{6!} + d_1\langle s\rangle\frac{\langle s^5\rangle}{5!} + d_2 k_1\frac{\langle s^4\rangle}{4!} + k_3\frac{\langle s^3\rangle}{3!}\right] - \frac{1}{3}d_1 k_9\langle s\rangle + \frac{1}{3}k_1\frac{k_9}{\langle s\rangle} - \frac{1}{27}k_1\left(\frac{k_2}{\langle s\rangle}\right)^2 \\ &- \frac{4}{135}\left[\frac{\langle s^6\rangle}{6!} + d_1\langle s\rangle\frac{\langle s^5\rangle}{5!} + d_1 k_2\frac{\langle s^3\rangle}{3!} + d_2 k_{10}\frac{\langle s^2\rangle}{2!} + d_1 k_{11}\langle s\rangle\right] + \frac{1}{3}\frac{k_2}{\langle s\rangle}\left[\frac{1}{9}k_{10} + \frac{4}{45}k_4\right], \end{aligned}$$

$$k_1 = \frac{\langle s^2\rangle}{2} + d_1\langle s\rangle^2, \quad k_2 = \frac{\langle s^3\rangle}{3!} + d_1\langle s\rangle\frac{\langle s^2\rangle}{2}, \quad k_3 = d_1 k_2 + d_1 d_2 k_1\langle s\rangle,$$

$$k_4 = \frac{\langle s^4\rangle}{4!} + d_1\langle s\rangle\frac{\langle s^3\rangle}{3!} + d_2 k_1\frac{\langle s^2\rangle}{2} + k_3\langle s\rangle, \quad k_5 = \frac{\langle s^5\rangle}{5!} + d_1\langle s\rangle\frac{\langle s^4\rangle}{4!} + d_2 k_1\frac{\langle s^3\rangle}{3!} + k_3\frac{\langle s^2\rangle}{2} + d_2 k_4\langle s\rangle,$$

$$k_6 = d_3 k_2 + d_3 d_2 k_1\langle s\rangle, \quad k_7 = \frac{\langle s^4\rangle}{4!} + d_1\langle s\rangle\frac{\langle s^3\rangle}{3!} + d_2 k_1\frac{\langle s^2\rangle}{2} + k_6\langle s\rangle,$$

$$k_8 = \frac{\langle s^5\rangle}{5!} + d_1\langle s\rangle\frac{\langle s^4\rangle}{4!} + d_2 k_1\frac{\langle s^3\rangle}{3!} + k_6\frac{\langle s^2\rangle}{2} + d_2 k_7\langle s\rangle,$$

$$k_9 = \frac{1}{9}\left[\frac{\langle s^5\rangle}{5!} + d_1\langle s\rangle\frac{\langle s^4\rangle}{4!} + d_1 k_2\frac{\langle s^2\rangle}{2}\right] + \frac{4}{45}\left[\frac{\langle s^5\rangle}{5!} + d_1\langle s\rangle\frac{\langle s^4\rangle}{4!} + d_2 k_1\frac{\langle s^3\rangle}{3!} + k_3\frac{\langle s^2\rangle}{2}\right],$$

$$k_{10} = \frac{\langle s^4\rangle}{4!} + d_1\langle s\rangle\frac{\langle s^3\rangle}{3!} + d_1 k_2\langle s\rangle, \quad k_{11} = \frac{\langle s^5\rangle}{5!} + d_1\langle s\rangle\frac{\langle s^4\rangle}{4!} + d_1 k_2\frac{\langle s^3\rangle}{3!} + d_2 k_{10}\langle s\rangle,$$

with

$$d_1 = \frac{ca_1}{1 - ca_1}, \quad d_2 = \frac{ca_2}{1 - ca_2}, \quad d_3 = \frac{ca_3}{1 - ca_3}.$$

If transport is classical (that is, Σ_t is independent of s and raw moments of s are given as in Eq. (6)), then these equations reduce to the classical SP_N equations with anisotropic scattering given by [10]. If scattering is isotropic ($a_1 = a_2 = a_3 = 0$), then these equations reduce to the nonclassical SP_N equations with isotropic scattering given in [9].

4. VACUUM BOUNDARY CONDITIONS

This asymptotic analysis does not produce boundary conditions, so we show that the nonclassical SP_N equations with anisotropic scattering can be manipulated into a classical form with modified parameters. This is done so we can obtain an approximate representation for the boundary conditions using classical (Marshak) vacuum boundary conditions [9].

4.1. SP$_1$ Boundary Conditions

We define

$$\hat{\Sigma}_{t,1} = \left[\frac{\langle s^2\rangle}{2\langle s\rangle} + \frac{c\bar{\mu}_0}{1-c\bar{\mu}_0}\langle s\rangle\right]^{-1}, \quad \text{and} \quad \hat{\Sigma}_{a,1} = \frac{1-c}{\langle s\rangle}. \tag{37a}$$

Then, the nonclassical SP$_1$ equation with anisotropic scattering and vacuum boundary condition can be written as

$$-\frac{1}{3\hat{\Sigma}_{t,1}}\nabla^2\Phi(\boldsymbol{x}) + \hat{\Sigma}_{a,1}\Phi(\boldsymbol{x}) = Q(\boldsymbol{x}), \qquad \frac{1}{2}\Phi(\boldsymbol{x}) - \frac{1}{3\hat{\Sigma}_{t,1}}\boldsymbol{n}\cdot\nabla\Phi(\boldsymbol{x}) = 0. \tag{38}$$

4.2. SP$_2$ Boundary Conditions

We define

$$\hat{\Sigma}_{t,2} = -\frac{1}{3\alpha_1}, \quad \hat{\Sigma}_{a,2} = \frac{(1-c)}{\langle s\rangle}\frac{1-\gamma_1(1-c)}{1+\rho_1(1-c)}, \quad \hat{Q}_2(\boldsymbol{x}) = \frac{1-\gamma_1(1-c)}{1+\rho_1(1-c)}Q(\boldsymbol{x}), \tag{39}$$
$$\hat{\Phi}(\boldsymbol{x}) = \Phi(\boldsymbol{x}) + \rho_1\left[(1-c)\Phi(\boldsymbol{x}) - \langle s\rangle Q(\boldsymbol{x})\right].$$

Then, the nonclassical SP$_2$ equation with anisotropic scattering and vacuum boundary condition can be written as

$$-\frac{1}{3\hat{\Sigma}_{t,2}}\nabla^2\hat{\Phi}(\boldsymbol{x}) + \hat{\Sigma}_{a,2}\hat{\Phi}(\boldsymbol{x}) = \hat{Q}_2(\boldsymbol{x}), \qquad \frac{1}{2}\hat{\Phi}(\boldsymbol{x}) - \frac{1}{3\hat{\Sigma}_{t,2}}\boldsymbol{n}\cdot\nabla\hat{\Phi}(\boldsymbol{x}) = 0. \tag{40}$$

The scalar flux can be recovered using

$$\Phi(\boldsymbol{x}) = \frac{\hat{\Phi}(\boldsymbol{x}) + \rho_1\langle s\rangle Q(\boldsymbol{x})}{1+\rho_1(1-c)}. \tag{41}$$

4.3. SP$_3$ Boundary Conditions

We define

$$\hat{\Sigma}_{t,3} = -\frac{1}{3\alpha_1}, \quad \hat{\Sigma}_{a,3} = \frac{1-c}{\langle s\rangle}\frac{1}{1+\gamma_1(1-c)}, \quad \hat{\Sigma}_2 = \frac{4\left[1+\gamma_1(1-c)\right]\left[1-\gamma_2(1-c)\right]}{5\rho_1\langle s\rangle}, \tag{42}$$
$$\hat{\Sigma}_3 = \frac{27}{28}\frac{\rho_1\hat{\Sigma}_{t,3}}{\rho_2\left[1+\gamma_1(1-c)\right]-\rho_1}, \quad \hat{Q}_3(\boldsymbol{x}) = \frac{Q(\boldsymbol{x})}{1+\gamma_1(1-c)}, \quad \hat{\Phi}_2(\boldsymbol{x}) = \frac{\nu(\boldsymbol{x})}{1+\gamma_1(1-c)}.$$

Then, the nonclassical SP_3 equations with anisotropic scattering can be expressed as

$$-\frac{1}{3\hat{\Sigma}_{t,3}}\nabla^2\left[\Phi(\boldsymbol{x})+2\hat{\Phi}_2(\boldsymbol{x})\right]+\hat{\Sigma}_{a,3}\Phi(\boldsymbol{x})=\hat{Q}_3(\boldsymbol{x}), \tag{43a}$$

$$-\frac{1}{3\hat{\Sigma}_{t,3}}\nabla^2\left[\frac{2}{5}\Phi(\boldsymbol{x})+\left(\frac{4}{5}+\frac{27\hat{\Sigma}_{t,3}}{35\hat{\Sigma}_3}\hat{\Phi}_2(\boldsymbol{x})\right)\right]+\hat{\Sigma}_2\hat{\Phi}_2(\boldsymbol{x})=0, \tag{43b}$$

and the vacuum boundary conditions are

$$\frac{1}{2}\Phi(\boldsymbol{x})-\frac{1}{3\hat{\Sigma}_{t,3}}n\cdot\nabla\Phi(\boldsymbol{x})-\frac{2}{3\hat{\Sigma}_{t,3}}n\cdot\nabla\hat{\Phi}_2(\boldsymbol{x})+\frac{5}{8}\hat{\Phi}_2(\boldsymbol{x})=0, \tag{44a}$$

$$-\frac{1}{8}\Phi(\boldsymbol{x})+\frac{5}{8}\hat{\Phi}_2(\boldsymbol{x})-\frac{3}{7\hat{\Sigma}_3}n\cdot\nabla\hat{\Phi}_2(\boldsymbol{x})=0. \tag{44b}$$

We also note that if scattering is isotropic, these modified boundary conditions reduce to the Marshak boundary conditions used in [9]. If the total macroscopic cross section is also independent of s, then these modified vacuum boundary conditions reduce to the classical Marshak vacuum boundary conditions.

5. NUMERICAL RESULTS

The nonclassical SP_N equations with anisotropic scattering are validated numerically in slab geometry with a slab of half-length M against a nonclassical transport equation benchmark. To generate this nonclassical transport benchmark, a spectral method uses Laguerre polynomials to express Eq. (1) in the form of a system of classical transport equations, which then allows the solution of the resulting system of transport equations with conventional numerical methods. Details of this spectral method for nonclassical transport are given in [11]. The SP_N equations and the benchmark use vacuum boundary conditions, with the SP_N vaccum boundary conditions given by those generated in Section 4. We assume steady-state, monoenergetic transport with a uniform, isotropic source Q which spans the entire slab. A scaling parameter $\epsilon \ll 1$ is chosen, and the slab and its parameters are scaled as follows:

$$M=\frac{1}{\epsilon}=O(1/\epsilon),\ \Sigma_t=1=O(1),\ Q=\frac{2}{M^2}=O(\epsilon^2),\ 1-c=\frac{0.5}{M^2}=O(\epsilon^2). \tag{45}$$

These choices imply that the system becomes more diffusive as M increases (that is, as $\epsilon\to 0$).

To simulate nonclassical transport, a nonexponential free path length distribution with a heavier tail than an exponential distribution is chosen, and this nonexponential distribution is

$$p(s)=se^{-s}, \tag{46}$$

whose mth raw moment is $(m+1)!$. To approximate anisotropic scattering, the anisotropic scattering distribution given by Eq. (2) is expanded to $m=3$ in slab geometry, resulting in

$$P(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')=\frac{1}{2}\left[1-\frac{3}{10}\mu_0-\frac{1}{4}(3\mu_0^2-1)+\frac{1}{5}(5\mu_0^3-3\mu_0)\right], \tag{47}$$

where $a_0=1$, $a_1=-1/10$, $a_2=-1/10$, and $a_3=2/35$ were chosen.

The transport benchmark and the nonclassical SP_1, SP_2, and SP_3 equations with anisotropic scattering employing Eqs. (46) and (47) are used to estimate the scalar flux in the slab. Figure 1 displays the relative percent error of each SP_N solution of the flux at the slab center ($x = 0$) against the benchmark solution. The figure demonstrates that the nonclassical SP_N equations with anisotropic scattering become more accurate as the system becomes more diffusive. The figure also shows that, as expected, the SP_3 equation is the most accurate since it contains the most information about the nonclassical nature of the particle transport and about the probability of anisotropic scattering which occurs in the slab.

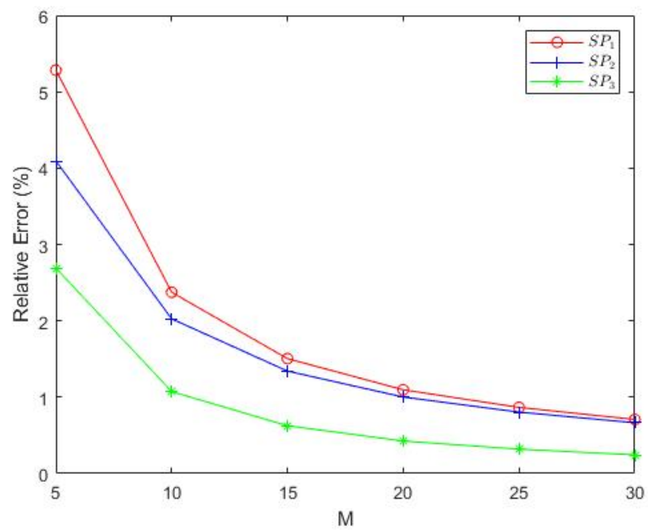

Figure 1: Relative Percent Error at the Center of the Slab

6. CONCLUSIONS

For the first time, the nonclassical SP_2 and SP_3 equations with anisotropic scattering have been explicitly derived. They were derived from a novel method which can be used to derive any of the nonclassical SP_N equations with anisotropic scattering. These equations were expressed in modified forms so that vacuum boundary conditions could be used. These modified forms of the nonclassical SP_N equations with anisotropic scattering with their vacuum boundary conditions were then validated in slab geometry. Parameters of the slab were chosen so that particle transport became more diffusive as the width of the slab increased. These scalar flux estimates were compared to the scalar flux computed by a transport benchmark, and the results showed that the nonclassical SP_N equations with anisotropic scattering became more accurate as the system became more diffusive.

The nonclassical SP_N equations with anisotropic scattering are generalizations of both the nonclassical SP_N equations with isotropic scattering and the classical SP_N equations with anisotropic scattering. Therefore, they can provide accurate estimations of particle transport in diffusive regimes in which nonclassical transport and anisotropic scattering are present. It is important to point out that, without boundary and interface conditions, the nonclassical SP_N equations with anisotropic scattering cannot model truly heterogeneous systems; currently, these equations can only model a homogeneous system with statistical properties identical to the heterogeneous system of interest.

Therefore, performing a variational analysis to derive these equations with appropriate boundary and interface conditions is a necessary future goal.

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