Derivation of a Multigroup Diffusion Equation for Nonclassical Problems

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ABSTRACT

We have derived an asymptotic approximation to the nonclassical energy-dependent transport equation with isotropic scattering. This approximation reduces to the classical multigroup diffusion equation under the assumption of classical transport, and therefore it consists of a generalization of the classical theory. The nonclassical multigroup diffusion equation can be implemented in existing multigroup diffusion codes since it preserves the same form of the classical equation but with modified parameters. We present analytical solutions to the nonclassical multigroup diffusion equation for three test problems in an one-dimensional (1-D) spatially periodic diffusive system consisting of alternating solid and void layers randomly placed along the x-axis. To assess the accuracy of these solutions, we compare against benchmark results obtained by (i) generating a large number of physical realizations of the system, (ii) numerically solving the (classical) transport equation in each realization, and (iii) ensemble-averaging the solutions over all physical realizations. The solution of the nonclassical multigroup diffusion equation asymptotically converges to the benchmark numerical solutions as the system becomes more diffusive, validating the analysis presented.

KEYWORDS: nonclassical transport, multigroup diffusion equation, random media

1. INTRODUCTION

The nonclassical theory of linear particle transport [1,2] was developed to address transport problems in which the particle flux is not attenuated exponentially. This can happen in certain inhomogeneous media in which the locations of the scattering centers are correlated. In these cases, the total cross section Σ_t is represented as dependent of the path length s (the distance traveled by the particle since its previous interaction). Applications of this nonclassical theory include neutron transport in reactor cores (cf. [3]), radiative transfer in atmospheric clouds (cf. [4]), and computer graphics (cf. [5]).

In this work we consider the steady-state, energy-dependent nonclassical linear transport equation with isotropic scattering. This equation is written as

$$\begin{aligned}&\frac{\partial\Psi}{\partial s}(s)+\boldsymbol{\Omega}\cdot\nabla\Psi(s)+\Sigma_t(s,E)\Psi(s)=\\&\qquad\frac{\delta(s)}{4\pi}\left[\int_0^\infty\int_{4\pi}\int_0^\infty c(E'\to E)\Sigma_t(s',E')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s',E')ds'd\boldsymbol{\Omega}'dE'+Q(\boldsymbol{x},E)\right],\end{aligned}\tag{1}$$

where $\Psi(s)=\Psi(\boldsymbol{x},\boldsymbol{\Omega},s,E)$ is the nonclassical angular flux, $c(E'\to E)dE'$ is the probability that, after colliding, a particle with energy in an interval dE' about E' will scatter into energy E, and $Q(\boldsymbol{x},E)$ is an energy-dependent isotropic source. The total cross section $\Sigma_t(s,E)$ is related to the particle free-path distribution by

$$p(s,E)=\Sigma_t(s,E)e^{-\int_0^s\Sigma_t(s',E)ds'}.\tag{2}$$

The one-speed (monoenergetic) nonclassical diffusion equation has been previously derived using different asymptotic approaches [1,2,6]. However, to our knowledge, this is the first time the nonclassical *multigroup* diffusion equation is explicitly presented and analyzed, generalizing the previous result by explicitly including energy dependence through the multigroup method. In order to assess the accuracy of this approach, we compare it against a benchmark solution for a two-group transport problem in a random periodic slab. This benchmark solution is obtained numerically by ensemble-averaging the solutions of the transport equation over a large number of physical realizations of the periodic random system. The results validate our analysis, confirming that the nonclassical multigroup diffusion equation generates a solution that asymptotically approaches that of the transport problem as the system becomes more diffusive.

The remainder of this paper is organized as follows. Section 2 details the asymptotic analysis used to derive the nonclassical multigroup diffusion equation. In Section 3, we (i) define the test problem and the different choices of parameters; (ii) discuss the model used to solve the test problems; and (iii) present and analyze the results. We close the paper in Section 4 with a discussion of the results and intended future work.

2. ASYMPTOTIC ANALYSIS

The multigroup approximation of transport theory is used to discretize the energy variable E into G energy groups. Let us consider the multigroup representation of the nonclassical transport equation (1) in its initial value form:

$$\frac{\partial \vec{\Psi}}{\partial s}(s) + \boldsymbol{\Omega} \cdot \nabla \vec{\Psi}(s) + \underline{\underline{\Sigma_t}}(s) \vec{\Psi}(s) = 0, \quad s > 0, \tag{3a}$$

$$\vec{\Psi}(0) = \frac{1}{4\pi} \left[\int_{4\pi} \int_0^\infty \underline{c} \underline{\underline{\Sigma_t}}(s') \vec{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}', s') ds' d\boldsymbol{\Omega}' + \vec{Q}(\boldsymbol{x}) \right], \tag{3b}$$

where $\vec{\Psi}(s) = \vec{\Psi}(\boldsymbol{x}, \boldsymbol{\Omega}, s)$ is a G vector whose gth component is the angular flux of neutrons in group g, $\vec{\Psi}(0) = \lim_{s \to 0^+} \vec{\Psi}(\boldsymbol{x}, \Omega, s) = \vec{\Psi}(0^+)$, $\underline{\underline{\Sigma_t}}(s)$ is a $G \times G$ diagonal matrix, $\underline{c}$ is the scattering matrix (a $G \times G$ matrix), and $\vec{Q}(\boldsymbol{x})$ is a G vector. Without loss of generality, we will consider the equation for the last energy group $g = G$, given by

$$\frac{\partial \Psi_G}{\partial s}(s) + \boldsymbol{\Omega} \cdot \nabla \Psi_G(s) + \Sigma_{t,G}(s) \Psi_G(s) = 0, \quad s > 0, \tag{4a}$$

$$\Psi_G(0) = \frac{1}{4\pi} \left[\int_{4\pi} \int_0^\infty c_{G \to G} \Sigma_{t,G}(s') \Psi_G(\boldsymbol{x}, \boldsymbol{\Omega}', s') ds' d\boldsymbol{\Omega}' + Q_G(\boldsymbol{x}) \right]. \tag{4b}$$

For simplicity, we are not considering upscattering in this work. This implies that $c_{g' \to g} = 0 \; \forall \, g' > g$, which is the reason we only consider $c_{G \to G}$ in the equation above.

We will now perform an asymptotic analysis on Eqs. (4), following the one presented in [6]. We point out that *we will drop the subscripts* G and $G \to G$ from the next steps for clarity of notation.

Defining $0 < \varepsilon \ll 1$, we perform the following scaling [6]:

$$\Sigma_t(s) = \frac{\Sigma_t(s/\varepsilon)}{\varepsilon}, \tag{5a}$$

$$c = 1 - \varepsilon^2 \kappa, \tag{5b}$$

$$Q(\boldsymbol{x}) = \varepsilon q(\boldsymbol{x}), \tag{5c}$$

where κ and q are $O(1)$. This scaling is consistent with the one used in [7] to obtain the multigroup classical SP$_N$ approximations for the multigroup classical transport equation. For $m = 1, 2, ...$ we define the m-th raw moment of the free-path distribution $p(s)$ for the energy group G as

$$\langle s^m \rangle = \int_0^\infty s^m p(s) ds, \tag{6}$$

where

$$p(s) = \Sigma_t(s)e^{-\int_0^s \Sigma_t(s')ds'}. \tag{7}$$

The following identity holds for $m = 1, 2, ...$:

$$\langle s^m \rangle = m \int_0^\infty s^{m-1} e^{-\int_0^s \Sigma_t(s')ds'} ds. \tag{8}$$

Moreover, using Eqs. (5a), (6), and (7), we can define $\langle s^m \rangle$ such that

$$\begin{aligned}\langle s^m \rangle &= \varepsilon^m \int_0^\infty \left(\frac{s}{\varepsilon}\right)^m \frac{\Sigma_t(s/\varepsilon)}{\varepsilon} e^{-\int_0^s \frac{\Sigma_t(s'/\varepsilon)}{\varepsilon} ds'} ds \\ &= \varepsilon^m \int_0^\infty s^m \Sigma_t(s) e^{-\int_0^s \Sigma_t(s')ds'} ds \\ &= \varepsilon^m \langle s^m \rangle_\varepsilon.\end{aligned} \tag{9}$$

With this scaling, Eqs. (4) become

$$\begin{aligned}&\frac{\partial \Psi}{\partial s}(s) + \boldsymbol{\Omega} \cdot \nabla \Psi(s) + \frac{1}{\varepsilon}\Sigma_t(s/\varepsilon)\Psi(s) = 0, \quad s > 0, \\ &\Psi(0) = \frac{1}{4\pi}\left[\int_{4\pi}\int_0^\infty (1-\varepsilon^2\kappa)\Sigma_t(s'/\varepsilon)\Psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\boldsymbol{\Omega}' + \varepsilon q(\boldsymbol{x})\right].\end{aligned}$$

Next, we define

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, \varepsilon s) \equiv \Psi_\varepsilon(\boldsymbol{x}, \boldsymbol{\Omega}, s),$$

which satisfies

$$\begin{aligned}&\frac{\partial \Psi_\varepsilon}{\partial s}(s) + \varepsilon\boldsymbol{\Omega} \cdot \nabla \Psi_\varepsilon(s) + \Sigma_t(s)\Psi_\varepsilon(s) = 0, \quad s > 0, \\ &\Psi_\varepsilon(0) = \frac{1}{4\pi}\left[\int_{4\pi}\int_0^\infty (1-\varepsilon^2\kappa)\Sigma_t(s')\Psi_\varepsilon(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\boldsymbol{\Omega}' + \varepsilon q(\boldsymbol{x})\right].\end{aligned}$$

Then, we define

$$\Psi_\varepsilon(\boldsymbol{x}, \boldsymbol{\Omega}, s) \equiv \psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)\frac{e^{-\int_0^s \Sigma_t(s')ds'}}{\varepsilon\langle s \rangle_\varepsilon},$$

such that ψ satisfies

$$\frac{\partial \psi}{\partial s}(s) + \varepsilon\boldsymbol{\Omega} \cdot \nabla \psi = 0, \quad s > 0, \tag{10a}$$

$$\psi(0) = \frac{1}{4\pi}\left[\int_{4\pi}\int_0^\infty (1-\varepsilon^2\kappa)p(s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\boldsymbol{\Omega}' + \varepsilon^2\langle s \rangle_\varepsilon q(\boldsymbol{x})\right]. \tag{10b}$$

We remark that the corresponding scalar flux can be recovered by

$$\begin{aligned}\Phi(\boldsymbol{x}) &= \int_{4\pi}\int_0^\infty \varepsilon\Psi_\varepsilon(\boldsymbol{x}, \boldsymbol{\Omega}, s)dsd\boldsymbol{\Omega} \\ &= \int_{4\pi}\int_0^\infty \psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)\frac{e^{-\int_0^s \Sigma_t(s')ds'}}{\langle s \rangle_\varepsilon}dsd\Omega.\end{aligned} \tag{11}$$

Integrating Eq. (10a) over $0 < s' < s$ and using Eq. (10b), we obtain

$$\left(I + \varepsilon\boldsymbol{\Omega} \cdot \nabla \int_0^s (\cdot)ds\right)\psi = \frac{1}{4\pi}\left[\int_0^\infty (1-\varepsilon^2\kappa)p(s')\varphi(\boldsymbol{x}, s')ds' + \varepsilon^2\langle s \rangle_\varepsilon q(\boldsymbol{x})\right], \tag{12}$$

where

$$\varphi(\boldsymbol{x}, s) = \int_{4\pi} \psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) d\Omega.$$

Inverting the operator on the left-hand side of Eq. (12) and expanding it in a power series, we obtain

$$\psi = \Big(\sum_{n=0}^{\infty} (-\varepsilon)^n \Big(\boldsymbol{\Omega} \cdot \nabla \int_0^s (\cdot) ds\Big)^n\Big) \times \frac{1}{4\pi} \left[\int_0^\infty (1 - \varepsilon^2 \kappa) p(s') \varphi(\boldsymbol{x}, s') ds' + \varepsilon^2 \langle s \rangle_\varepsilon q(\boldsymbol{x})\right]. \tag{13}$$

Let us define

$$\nabla_0 = \frac{1}{3} \nabla^2, \tag{14a}$$

$$\mathcal{B} = \nabla_0 \Big(\int_0^s (\cdot) ds\Big)^2. \tag{14b}$$

Then, using the identity [8]

$$\frac{1}{4\pi} \int_{4\pi} \Big(\boldsymbol{\Omega} \cdot \nabla \int_0^s (\cdot) ds\Big)^n d\Omega = \frac{1 + (-1)^n}{2} \frac{(3\mathcal{B})^{n/2}}{n+1},$$

for $n = 0, 1, 2, ...$, we integrate Eq. (13) over the unit sphere and obtain

$$\varphi = \Big(\sum_{n=0}^{\infty} \frac{1}{2n+1} (3\varepsilon^2 \mathcal{B})^n\Big) \times \left[\int_0^\infty (1 - \varepsilon^2 \kappa) p(s') \varphi(\boldsymbol{x}, s') ds' + \varepsilon^2 \langle s \rangle_\varepsilon q(\boldsymbol{x})\right].$$

Inverting the operator on the right-hand side of this equation and once again expanding it in a power series, we get

$$\Big(I - \varepsilon^2 \mathcal{B} - \frac{4\varepsilon^4}{5} \mathcal{B}^2 - \frac{44\varepsilon^6}{35} \mathcal{B}^3 + O(\varepsilon^8)\Big) \varphi = \int_0^\infty (1 - \varepsilon^2 \kappa) p(s') \varphi(\boldsymbol{x}, s') ds' + \varepsilon^2 \langle s \rangle_\varepsilon q(\boldsymbol{x}). \tag{15}$$

The solution of this equation is

$$\varphi(\boldsymbol{x}, s) = \Big(I + \varepsilon^2 \frac{s^2}{2!} \nabla_0 + \frac{9\varepsilon^4}{5} \frac{s^4}{4!} \nabla_0^2 + \frac{27\varepsilon^6}{7} \frac{s^6}{6!} \nabla_0^3 + O(\varepsilon^8)\Big) \phi(\boldsymbol{x}), \tag{16}$$

where

$$\phi(\boldsymbol{x}) = \sum_{n=0}^{\infty} \varepsilon^{2n} \phi_{2n}(\boldsymbol{x}),$$

with $\phi_{2n}(\boldsymbol{x})$ undetermined at this point. We multiply Eq. (16) by $e^{-\int_0^s \Sigma_t(s')ds'} / \langle s \rangle_\varepsilon$ and operate on it by $\int_0^\infty (\cdot) ds$. Using Eqs. (8), (9), and (11), we obtain an expression for the scalar flux:

$$\Phi(\boldsymbol{x}) = \Big(I + \varepsilon^2 \frac{\langle s^3 \rangle_\varepsilon}{3! \langle s \rangle_\varepsilon} \nabla_0 + \frac{9\varepsilon^4}{5} \frac{\langle s^5 \rangle_\varepsilon}{5! \langle s \rangle_\varepsilon} \nabla_0^2 + \frac{27\varepsilon^6}{7} \frac{\langle s^7 \rangle_\varepsilon}{7! \langle s \rangle_\varepsilon} \nabla_0^3 + O(\varepsilon^8)\Big) \phi(\boldsymbol{x}).$$

Hence, we can write

$$\int_0^\infty p(s) \varphi(\boldsymbol{x}, s) ds = \left(\sum_{n=0}^{\infty} \varepsilon^{2n} U_n \nabla_0^n\right) \Phi(\boldsymbol{x}), \tag{17}$$

with

$$
\begin{aligned}
U_0 &= 1,\\
U_1 &= \frac{\langle s^2\rangle_\varepsilon}{2!} - \frac{\langle s^3\rangle_\varepsilon}{3!\langle s\rangle_\varepsilon},\\
U_2 &= \frac{9}{5}\left[\frac{\langle s^4\rangle_\varepsilon}{4!} - \frac{\langle s^5\rangle_\varepsilon}{5!\langle s\rangle_\varepsilon}\right] - \frac{\langle s^3\rangle_\varepsilon}{3!\langle s\rangle_\varepsilon}U_1,\\
U_3 &= \frac{27}{7}\left[\frac{\langle s^6\rangle_\varepsilon}{6!} - \frac{\langle s^7\rangle_\varepsilon}{7!\langle s\rangle_\varepsilon}\right] - \frac{9}{5}\frac{\langle s^5\rangle_\varepsilon}{5!\langle s\rangle_\varepsilon}U_1 - \frac{\langle s^3\rangle_\varepsilon}{3!\langle s\rangle_\varepsilon}U_2,\\
&\vdots
\end{aligned}
$$

Equation (15) can be rewritten as

$$
\left(\sum_{n=0}^{\infty}\varepsilon^{2n}V_n\nabla_0^n\right)\Phi(\boldsymbol{x}) = (1-\varepsilon^2\kappa)\left(\sum_{n=0}^{\infty}\varepsilon^{2n}U_n\nabla_0^n\right)\Phi(\boldsymbol{x}) + \varepsilon^2\langle s\rangle_\varepsilon q(\boldsymbol{x}), \tag{18}
$$

where

$$
\begin{aligned}
V_0 &= 1,\\
V_1 &= -\frac{\langle s^3\rangle_\varepsilon}{3!\langle s\rangle_\varepsilon}V_0,\\
V_2 &= -\frac{9}{5}\frac{\langle s^5\rangle_\varepsilon}{5!\langle s\rangle_\varepsilon}V_0 - \frac{\langle s^3\rangle_\varepsilon}{3!\langle s\rangle_\varepsilon}V_1,\\
V_3 &= -\frac{27}{7}\frac{\langle s^7\rangle_\varepsilon}{7!\langle s\rangle_\varepsilon}V_0 - \frac{9}{5}\frac{\langle s^5\rangle_\varepsilon}{5!\langle s\rangle_\varepsilon}V_1 - \frac{\langle s^3\rangle_\varepsilon}{3!\langle s\rangle_\varepsilon}V_2,\\
&\vdots
\end{aligned}
$$

Finally, rearranging the terms in Eq. (18) we get

$$
\left(\sum_{n=0}^{\infty}\varepsilon^{2n}[W_{n+1}\nabla_0^{n+1} + \kappa U_n\nabla_0^n]\right)\Phi(\boldsymbol{x}) = \langle s\rangle_\varepsilon q(\boldsymbol{x}), \tag{19}
$$

where $W_n = V_n - U_n$.
We discard the terms of $O(\varepsilon^2)$ in Eq. (19) and rewrite the equation as

$$
W_1\nabla_0\Phi(\boldsymbol{x}) + \kappa\Phi(\boldsymbol{x}) = \langle s\rangle_\varepsilon q(\boldsymbol{x}).
$$

Using Eq.(14a), we get

$$
-\frac{1}{6}\frac{\langle s^2\rangle_\varepsilon}{\langle s\rangle_\varepsilon}\nabla^2\Phi(\boldsymbol{x}) + \frac{\kappa}{\langle s\rangle_\varepsilon} = q(\boldsymbol{x}).
$$

Finally, we multiply this equation by ε and use Eqs. (5) and (9) to revert to the original unscaled parameters. We can now reintroduce the subscripts G and $G \to G$ to write

$$
-\frac{1}{6}\frac{\langle s^2\rangle_G}{\langle s\rangle_G}\nabla^2\Phi_G(\boldsymbol{x}) + \frac{1}{\langle s\rangle_G}\Phi_G(\boldsymbol{x}) = \frac{c_{G\to G}}{\langle s\rangle_G}\Phi_G(\boldsymbol{x}) + Q_G(\boldsymbol{x})\,, \tag{20}
$$

which is the multigroup nonclassical diffusion equation with isotropic scattering for the energy group $g = G$. At last, we can generalize Eq. (20) for each energy group g as

$$
-\frac{1}{6}\frac{\langle s^2\rangle_g}{\langle s\rangle_g}\nabla^2\Phi_g(\boldsymbol{x}) + \frac{1}{\langle s\rangle_g}\Phi_g(\boldsymbol{x}) = \sum_{g'=1}^{G}\frac{c_{g'\to g}}{\langle s\rangle_{g'}}\Phi_{g'}(\boldsymbol{x}) + Q_g(\boldsymbol{x}), \qquad 1 \le g \le G. \tag{21}
$$

This is a system of G coupled diffusion equations in the G unknowns $\Phi_g(\boldsymbol{x})$, representing a multigroup nonclassical diffusion approximation to the nonclassical transport equation (1).

The multigroup m-th raw moment of the multigroup free-path distribution function $p_g(s)$ is defined as

$$\langle s^m \rangle_g = \int_0^\infty s^m p_g(s) ds, \quad p_g(s) = \Sigma_{t,g}(s) e^{-\int_0^s \Sigma_{t,g}(s')ds'}, \qquad 1 \leq g \leq G. \tag{22}$$

Thus, the multigroup nonclassical diffusion equation is an asymptotic approximation to the nonclassical transport equation with an $O(\varepsilon^2)$ error. We note that this asymptotic analysis requires that the first two moments of $p_g(s)$ exist for all energy groups g [6].

The asymptotic analysis presented in this paper does not provide boundary conditions. However, we can overcome this limitation by demonstrating that the multigroup nonclassical diffusion equation can be transformed into a classical form with adjusted parameters. By doing so, we can apply classical (Marshak) vacuum boundary conditions [9]. Moreover, this approach shows that the multigroup nonclassical diffusion equation can be implemented in existing multigroup diffusion codes with minimal effort.

Let us define

$$\begin{aligned}
\widehat{\Sigma}_{t,g} &= 2\frac{\langle s \rangle_g}{\langle s^2 \rangle_g}, \qquad 1 \leq g \leq G, \\
\widehat{\Sigma}_{a,g} &= \frac{1 - c_{g\to g}}{\langle s \rangle_g}, \qquad 1 \leq g \leq G, \\
\widehat{\Sigma}_{s,g'\to g} &= \frac{c_{g'\to g}}{\langle s \rangle_{g'}}, \qquad 1 \leq g \leq G.
\end{aligned}$$

Then, the multigroup nonclassical diffusion equation with isotropic scattering (Eq. (21)) can be written in classical form as

$$-\frac{1}{3\widehat{\Sigma}_{t,g}} \nabla^2 \Phi_g(\boldsymbol{x}) + \widehat{\Sigma}_{a,g} \Phi_g(\boldsymbol{x}) = \sum_{\substack{g'=1 \\ g' \neq g}}^{G} \widehat{\Sigma}_{s,g'\to g} \Phi_{g'}(\boldsymbol{x}) + Q_g(\boldsymbol{x}), \qquad 1 \leq g \leq G. \tag{23a}$$

The vacuum boundary conditions for this equation are given by [6]

$$\frac{1}{2}\Phi_g(\boldsymbol{x}) - \frac{1}{3\widehat{\Sigma}_{t,g}} \mathbf{n} \cdot \nabla \Phi_g(\boldsymbol{x}) = 0, \qquad 1 \leq g \leq G. \tag{23b}$$

If the multigroup free-path distribution is given by the exponential $p_g(s) = \Sigma_{t,g} e^{-\Sigma_{t,g} s}$, the raw moments defined in Eq. (22) yield the classical form

$$\langle s^m \rangle_g = \int_0^\infty s^m \Sigma_{t,g} e^{-\Sigma_{t,g} s} ds = \frac{m!}{\Sigma_{t,g}^m}, \qquad 1 \leq g \leq G. \tag{24}$$

This implies that $\widehat{\Sigma}_{t,g} = \Sigma_{t,g}$, $\widehat{\Sigma}_{a,g} = \Sigma_{a,g}$, and $\widehat{\Sigma}_{s,g'\to g} = \Sigma_{s,g'\to g}$, and Eqs. (23) simplify to the classical multigroup diffusion equation with Marshak vacuum boundary conditions.

3. TEST PROBLEM AND NUMERICAL RESULTS

Numerical results in this work consider transport taking place in a 1-D finite random periodic slab in two energy groups ($G = 2$) with vacuum boundaries. The system is formed by a random segment of alternating layers of two distinct materials (labeled 1 and 2) periodically arranged. We assume material 1 to be the one in which particles can be born and collide, while material 2 is assumed to be void; a sketch of the periodic system is given in Figure 1 .

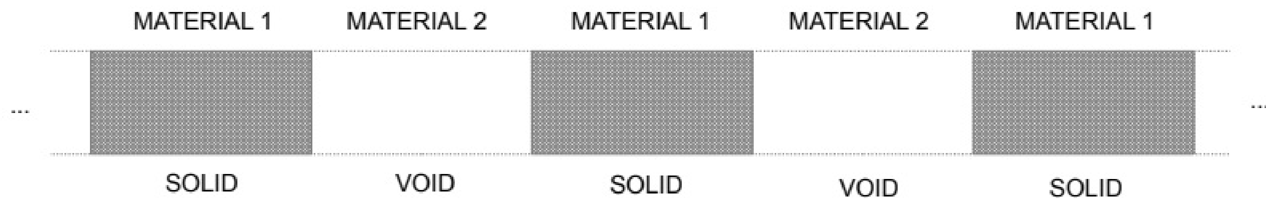

Figure 1: A sketch of the random periodic medium

The width of each layer is $0.5\,cm$. The total width of the system is given by X = $2M$, where M is a positive integer number. Vacuum boundary conditions are assigned at $x = 0$ and $x = X$. Cross sections and sources of material 1 and 2 for each energy group g are given in Table 1, and the scattering matrix is given by

$$\begin{bmatrix} c_{1\to1} & c_{1\to2} \\ c_{2\to1} & c_{2\to2} \end{bmatrix} = \begin{bmatrix} 0.999 - \frac{0.1}{M^2} & 0.001 \\ 0 & 1 - \frac{0.1}{M^2} \end{bmatrix} \tag{25}$$

where $c_{2\to1} = 0$ because there is no upscattering in this problem. With this choice of parameters one can see that, as M increases, the 1-D system approaches the diffusive limit [6].

Table 1: Total cross section (cm^{-1}) and isotropic source ($cm^{-3}s^{-1}$) of materials 1 and 2

g	$\Sigma_{t1,g}$	$Q_{1,g}$	$\Sigma_{t2,g}$	$Q_{2,g}$
1	0.5	$\frac{0.2}{M^2}$	0	0
2	1.0	$\frac{0.2}{M^2}$	0	0

Taking into account the parameters considered in this summary, we have calculated the first and second moments of the ensemble-averaged free-path distribution for each energy group g, given in Table 2, using [10]

$$\langle s \rangle_g = \frac{2}{\Sigma_{t1,g}}, \qquad g = 1, 2, \tag{26a}$$

$$\langle s^2 \rangle_g = \frac{6}{\Sigma_{t1,g}^2} + \frac{1}{2\Sigma_{t1,g}} \left(\frac{e^{0.5\Sigma_{t1,g}} + 1}{e^{0.5\Sigma_{t1,g}} - 1} \right), \qquad g = 1, 2. \tag{26b}$$

Table 2: First and second moments of $p_g(s)$.

g	$\langle s \rangle_g$ (cm)	$\langle s^2 \rangle_g$ (cm^2)
1	4.0	32.04162332837560
2	2.0	8.041494082536797

Because we are conducting simulations within a 1-D slab, we solve the one-dimensional form of Eqs. (23):

$$-\frac{1}{3\widehat{\Sigma}_{t,1}} \frac{d^2}{dx^2} \Phi_1(x) + \widehat{\Sigma}_{a,1} \Phi_1(x) = Q_1(x)\,, \tag{27a}$$

$$-\frac{1}{3\widehat{\Sigma}_{t,2}} \frac{d^2}{dx^2} \Phi_2(x) + \widehat{\Sigma}_{a,2} \Phi_2(x) = \widehat{\Sigma}_{s,1\to2} \Phi_1(x) + Q_2(x)\,, \tag{27b}$$

with the one-dimensional form of the vacuum boundary conditions

$$\frac{1}{2}\Phi_g(0) + \frac{1}{3\widehat{\Sigma}_{t,g}}\frac{d}{dx}\Phi_g(0) = 0, \qquad g = 1, 2\,, \tag{27c}$$

$$\frac{1}{2}\Phi_g(X) - \frac{1}{3\widehat{\Sigma}_{t,g}}\frac{d}{dx}\Phi_g(X) = 0, \qquad g = 1, 2\,. \tag{27d}$$

3.1. Benchmark Model

To generate benchmark results for comparison, we used the same procedure presented in [10]. In this procedure, we obtain a physical realization of the system by choosing a continuous segment of two full layers (one of each material) and randomly placing the coordinate $x = 0$ in this segment. Given this fixed realization of the system, the cross sections and source are now deterministic functions of space.

We solve the classical multigroup transport equation numerically for this realization using (i) the standard discrete ordinate method with a 16-point Gauss-Legendre quadrature set (S_{16}); and (ii) diamond spatial differencing scheme with mesh interval $\Delta x = 2^{-7}$. For each test problem, this procedure is repeated for $2\ell/\Delta x = 128$ different realizations of the periodic system obtained by shifting the x-coordinates by Δx each time. Finally, we calculate the ensemble-averaged scalar flux $\langle\Phi\rangle_g(x)$ by averaging the resulting scalar fluxes over all 128 physical realizations.

In all problems, differences in the numerical results for $\langle\Phi\rangle_g(x)$ were negligible when increasing the number of mesh intervals, the number of realizations, and the n-th order of the Gauss-Legendre quadrature; thus, we have concluded that these benchmark results are adequately accurate for the scope of this work.

3.2. Numerical Results

We present solutions for increasing values of M: 15, 30, and 60. The scalar fluxes plotted in Figures 2, 3, and 4 show that the solution to the one-dimensional nonclassical multigroup diffusion equation (27) asymptotically approaches the benchmark transport solution as M increases and the system approaches the diffusive limit, as predicted by our asymptotic analysis.

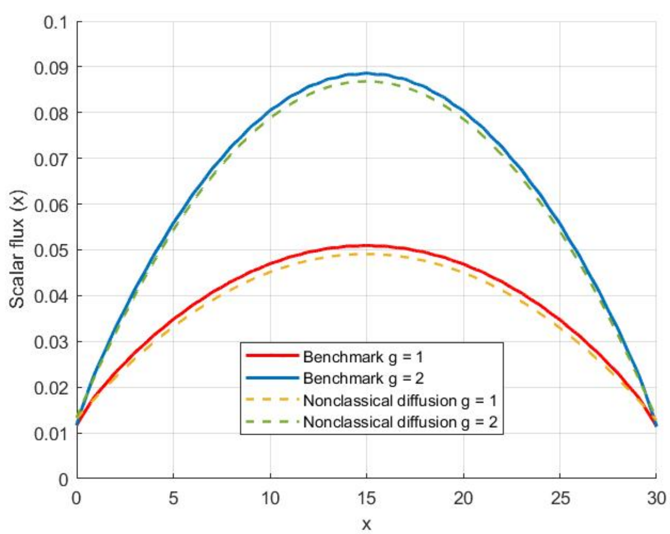

Figure 2: Scalar fluxes ($cm^{-2}s^{-1}$) obtained with M = 15.

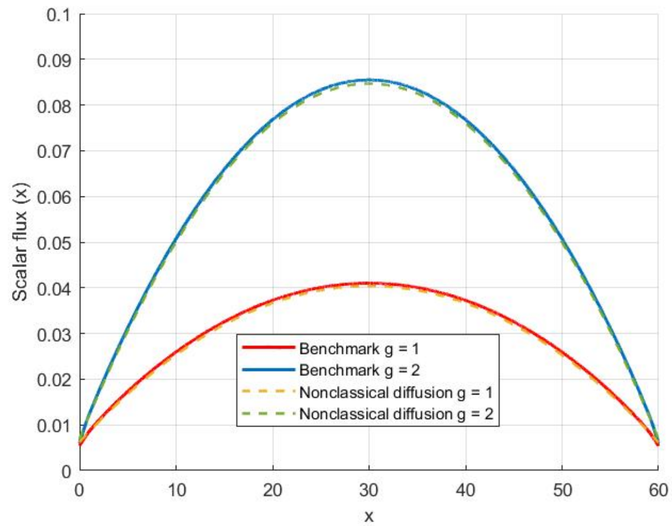

Figure 3: Scalar fluxes ($cm^{-2}s^{-1}$) obtained with M = 30.

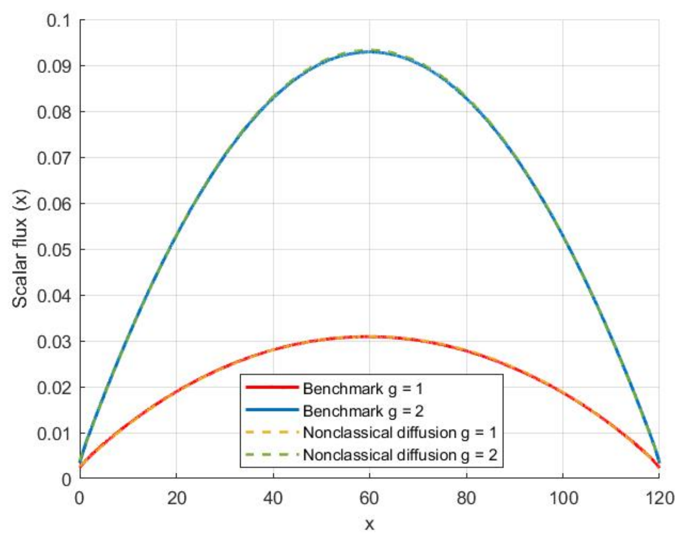

Figure 4: Scalar fluxes ($cm^{-2}s^{-1}$) obtained with M = 60.

4. DISCUSSION

This paper introduces a multigroup diffusion approximation for the multigroup nonclassical transport equation with isotropic scattering using an asymptotic analysis. This approximation simplifies to the classical multigroup diffusion equation under the assumption of classical transport. To the best of our knowledge, this is the first explicit derivation of a multigroup generalization to the monoenergetic nonclassical diffusion equation.

It is important to note that the asymptotic analysis used here has a constraint: the first two raw moments of the multigroup free-path distribution $p_g(s)$ must be finite. While the analysis does not provide boundary conditions, we demonstrate that the nonclassical multigroup diffusion equation can be transformed into a classical form with adjusted parameters. As a result, we can use Marshak vacuum boundary conditions to generate numerical results. The significant advantage of this method is that the nonclassical multigroup diffusion equation can be implemented in current multigroup diffusion codes.

Theoretical predictions were validated for a 1-D random periodic system. These findings provide a foundation for gaining a more comprehensive understanding of the diffusive behavior of nonclassical transport theory. In future work, we will perform numerical simulations in nonclassical multi-dimensional systems and investigate its accuracy for different choices of nonexponential path length distributions $p_g(s)$. In addition, we plan to simulate various test problems and compare our findings to those obtained using atomic mix diffusion and nonclassical Monte Carlo models. We will also expand the analysis to include linearly anisotropic scattering.

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