Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications
Palais des Papes, Avignon, France, September 12-15, 2005, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2005)

PARTICLE TRANSPORT IN THE 1-D DIFFUSIVE ATOMIC MIX LIMIT

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ABSTRACT

A multiple length-scale asymptotic analysis shows that 1-D diffusive heterogeneous-media transport problems are accurately modeled by the atomic mix approximation when the optical widths of the "chunks" of different materials are $O(1)$. (The atomic mix approximation is commonly known to be valid only when the chunks of different materials are optically thin.) The analysis also shows that for the same class of problems, the *Standard*, or *Levermore-Pomraning (LP)* model does not have the correct asymptotic behavior. Numerical results are given that validate the theoretical predictions.

KEYWORDS: particle transport, diffusion, atomic mix

1. INTRODUCTION

The *atomic mix approximation* is a simple, classic, and widely-used model for particle transport in a heterogeneous physical system consisting of two or more materials in which the "chunks" of the various materials are optically thin [1,2]. This approximation consists of replacing, in the transport equation, the spatially-variable cross sections by their volume-averages. Dumas and Golse [2] have recently proved that the atomic mix approximation is an asymptotic limit of the particle transport equation as the chunk widths limit to zero. This is precisely the limit in which the atomic mix approximation is commonly understood to be valid.

The *diffusion approximation* is an altogether different classic model, for particle transport in a physical system in which absorption and sources are weak and the solution varies slowly over the distance of a mean free path. The diffusion equation has long been known to be an asymptotic limit of the transport equation [3-5].

In this paper, we consider 1-D transport problems that combine features of both of these asymptotic limits. In particular, we assume that:

1. The physical system is *heterogeneous*, consisting of chunks of two materials. It is not necessary to know the locations of the boundaries of the chunks, but it is necessary to know the cross sections for each material and the volume fractions of the two materials in the system. Unlike the conventional atomic mix approximation, the chunks are not required to be optically thin; they can be on the order of a mean free path in thickness (or smaller).

2. The physical system is optically thick, and at each spatial point, absorption and sources are weak. In a global sense, the system is *diffusive*.

3. These two assumptions imply that the number of material chunks in the system is large. The structure of the system (in terms of the location of the chunks) can be either random or not-random (e.g., periodic).

In this paper, we show that for the above 1-D *diffusive atomic mix* problems, the solution of the particle transport equation is well-approximated by the solution of the atomic mix diffusion equation. [This is the conventional diffusion equation, whose coefficients are based on the atomic mix (volume-averaged) cross sections.] In effect, the diffusive atomic mix limit considered in this paper is one in which the asymptotic diffusion and atomic mix approximations are *both* applied – except that the material chunks are not required to be optically thin. To our knowledge, this is the first demonstration that the atomic mix approximation is valid for a class of problems in which the material chunks are not optically thin. A preliminary version of this work was recently published [6]. In the present paper, we provide more analytic details, and we give numerical results that confirm our theoretical predictions.

We also in this paper consider the *Standard* or *Levermore-Pomraning (LP)* approximation [1,7-10] in the diffusive atomic mix limit. The LP equations are a well-known generalization of the atomic mix approximation to systems in which the chunk widths are not optically thin. The LP model is known to be accurate for problems with (i) weak scattering, and (ii) a Markovian distribution of chord lengths across material chunks. However, numerical experiments have indicated that the LP model is inaccurate for diffusive systems [10]. In this paper, we show that in the diffusive atomic mix limit, the LP model reduces to a diffusion equation with an incorrect diffusion coefficient. This theoretically explains the inaccuracies observed in LP simulations for diffusive problems.

Finally, we include in this paper computational results that validate our theoretical predictions. These simulations demonstrate that for transport problems in the diffusive atomic mix limit, (i) the solution of the transport equation limits to the solution of the atomic mix diffusion equation, and (ii) the solution of the LP equations limit to the solution of a physically incorrect (but theoretically-predicted) diffusion equation. In all cases, the numerical results closely agree with the predictions of the asymptotic theory.

The remainder of this paper is organized as follows. In Sec. 2 we present the asymptotic theory for the transport equation, and in Sec. 3 we apply a similar asymptotic theory to the LP equations. In Sec. 4 we present numerical results that confirm the theoretical predictions. We conclude with a brief discussion in Sec. 5.

2. ASYMPTOTIC ANALYSIS OF THE TRANSPORT EQUATION

We consider the following 1-D transport problem, with vacuum boundaries, and space-dependent cross sections and source:

$$\mu \frac{\partial \Psi}{\partial x}(x,\mu) + \Sigma_t(x)\Psi(x,\mu) = \frac{\Sigma_s(x)}{2}\int_{-1}^{1}\Psi(x,\mu')d\mu' + \frac{Q(x)}{2} \ , \quad -X \le x \le X \ , \ -1 \le \mu \le 1 \ , \tag{2.1a}$$

$$\Psi(-X,\mu) = 0 \ , \ \ 0 < \mu \le 1 \ , \tag{2.1b}$$

$$\Psi(X,\mu) = 0 \ , \ \ -1 \le \mu < 0 \ . \tag{2.1c}$$

The physical system $-X \le x \le X$ consists of layers (chunks) of distinct materials. We assume:

1. The widths of the layers are comparable to (or small compared to) a mean free path.

2. The spatial variable x is scaled so that a typical chunk width and a typical mean free path are $O(1)$. [Thus, $\Sigma_t = O(1)$.]

3. The system is optically thick. Thus, the dimensionless parameter

$$\varepsilon \equiv \frac{\text{typical width of a chunk}}{\text{width of the system}} = \frac{1}{\text{number of chunks}} \tag{2.2a}$$

is small, and

$$2X = \text{ the system width } = O\left(\frac{1}{\varepsilon}\right) \ . \tag{2.2b}$$

4. At all spatial points, absorption is weak. We express this by writing the absorption cross section as

$$\Sigma_t(x) - \Sigma_s(x) = \Sigma_a(x) = \varepsilon^2 \sigma_a(x) \ , \tag{2.3}$$

where $\sigma_a(x) = O(1)$.

5. For convenience, the source is scaled so that the infinite-medium solution is $O(1)$. We express this by writing

$$Q(x) = \varepsilon^2 q(x) \ , \tag{2.4}$$

where $q(x) = O(1)$.

6. The flux depends on two spatial variables: the *fast* spatial variable x, which describes "rapid" variations on the order of a mean free path or a chunk width, and a new *slow* spatial variable

$$z = \varepsilon x \ , \tag{2.5}$$

which describes slowly-varying spatial variations in the flux over the $O(1/\varepsilon)$ optical width of the system. We express this assumption by writing

$$\Psi(x, \mu) = \psi(x, z, \mu) \ , \tag{2.6a}$$

which implies:

$$\frac{\partial \Psi}{\partial x}(x, \mu) = \frac{\partial \psi}{\partial x}(x, z, \mu) + \varepsilon \frac{\partial \psi}{\partial z}(x, z, \mu) \ . \tag{2.6b}$$

Introducing Eqs. (2.3)-(2.6) into Eq. (2.1a), we obtain the following scaled transport equation:

$$\begin{aligned} \mu \frac{\partial \psi}{\partial x}(x, z, \mu) + \varepsilon \mu \frac{\partial \psi}{\partial z}(x, z, \mu) + \Sigma_t(x) \psi(x, z, \mu) \\ = \frac{\Sigma_t(x) - \varepsilon^2 \sigma_a(x)}{2} \int_{-1}^{1} \psi(x, z, \mu') d\mu' + \varepsilon^2 \frac{q(x)}{2} \ . \end{aligned} \tag{2.7}$$

To asymptotically solve this equation, we assume the ansatz:

$$\psi(x, z, \mu) = \sum_{n=0}^{\infty} \varepsilon^n \psi_n(x, z, \mu) \ , \tag{2.8}$$

in which $\varepsilon \ll 1$, and x and z are treated as independent variables. Introducing Eq. (2.8) into Eq. (2.7) and equating the coefficients of different powers of ε, we obtain for $n \geq 0$:

$$\mu \frac{\partial \psi_n}{\partial x}(x,z,\mu) + \Sigma_t(x) \left[\psi_n(x,z,\mu) - \frac{1}{2} \int_{-1}^{1} \psi_n(x,z,\mu') d\mu' \right] = -\mu \frac{\partial \psi_{n-1}}{\partial z}(x,z,\mu) - \frac{\sigma_a(z)}{2} \int_{-1}^{1} \psi_{n-2}(x,z,\mu') d\mu' + \delta_{n,2} \frac{q(x)}{2} \quad , \tag{2.9}$$

where $\psi_{-1} = \psi_{-2} = 0$. These equations are solved first for $n = 0$, then $n = 1$, etc.

The $n = 0$ equation,

$$\mu \frac{\partial \psi_0}{\partial x}(x,z,\mu) + \Sigma_t(x) \left[\psi_0(x,z,\mu) - \frac{1}{2} \int_{-1}^{1} \psi_0(x,z,\mu') d\mu' \right] = 0 \quad , \tag{2.10}$$

is a purely-scattering transport equation. It has the following isotropic, bounded solution:

$$\psi_0(x,z,\mu) = \frac{1}{2} \phi_0(z) \quad , \tag{2.11}$$

where $\psi_0(z)$ is undetermined.

Eq. (2.9) for $n = 1$ becomes:

$$\mu \frac{\partial \psi_1}{\partial x}(x,z,\mu) + \Sigma_t(x) \left[\psi_1(x,z,\mu) - \frac{1}{2} \int_{-1}^{1} \psi_1(x,z,\mu') d\mu' \right] = -\frac{\mu}{2} \frac{d\phi_0}{dz}(z) \quad . \tag{2.12}$$

A particular solution of Eq. (2.12) is linear in μ:

$$\psi_{1,part}(x,z,\mu) = \psi_{10}(x,z) + \mu \psi_{11}(z) \quad . \tag{2.13}$$

Introducing Eq. (2.13) into Eq. (2.12) and equating the coefficients of μ^n for $n = 0$ and 1, we obtain two equations for ψ_{10} and ψ_{11}. These equations quickly yield the following particular solution:

$$\psi_{1,part}(x,z,\mu) = -\frac{1}{2} \left(g(x) + \frac{\mu}{\overline{\Sigma}_t} \right) \frac{d\phi_0}{dz}(z) \quad , \tag{2.14a}$$

where

$$g(x) = \int_{-X}^{x} \left(1 - \frac{\Sigma_t(x')}{\overline{\Sigma}_t} \right) dx' \quad , \tag{2.14b}$$

and

$$\overline{\Sigma}_t = \frac{1}{2X} \int_{-X}^{X} \Sigma_t(x') dx' = \text{ volume-averaged total cross section} \quad . \tag{2.14c}$$

The general solution of Eq. (2.12) is then:

$$\psi_1(x,z,\mu) = \frac{1}{2} \phi_1(z) - \frac{1}{2} \left(g(x) + \frac{\mu}{\overline{\Sigma}_t} \right) \frac{d\phi_0}{dz}(z) \quad , \tag{2.15}$$

where $\phi_1(z)$ is undetermined.

Next, Eq. (2.9) for $n = 2$ becomes:

$$\mu\frac{\partial\psi_2}{\partial x}(x,z,\mu) + \Sigma_t(x)\left[\psi_2(x,z,\mu) - \frac{1}{2}\int_{-1}^{1}\psi_2(x,z,\mu')d\mu'\right] \quad .$$
$$= -\mu\frac{\partial}{\partial z}\left[\frac{1}{2}\phi_1(z) - \frac{1}{2}\left(g(x) + \frac{\mu}{\overline{\Sigma}_t}\right)\frac{d\phi_0}{dz}(z)\right]$$
$$- \frac{\sigma_a(x)}{2}\phi_0(z) + \frac{q(x)}{2} \quad . \tag{2.16}$$

For a bounded solution of this equation to exist, the right side must satisfy a solvability condition, obtained by operating on Eq. (2.16) by $\frac{1}{2X}\int_{-X}^{X}\int_{-1}^{1}(\cdot)d\mu dx$. We obtain

$$\frac{1}{2X}\left[\int_{-1}^{1}\mu\psi_2(X,z,\mu)d\mu - \int_{-1}^{1}\mu\psi_2(-X,z,\mu)d\mu\right] = \frac{1}{3\overline{\Sigma}_t}\frac{d^2\phi_0}{dz^2}(z) - \overline{\sigma}_a\phi_0(z) + \overline{q} \quad , \tag{2.17a}$$

where

$$\overline{\sigma}_a = \frac{1}{2X}\int_{-X}^{X}\sigma_a(x)dx = \text{ volume-averaged absorption cross section} \quad , \tag{2.17b}$$

$$\overline{q} = \frac{1}{2X}\int_{-X}^{X}q(x)dx = \text{ volume-averaged interior source} \quad . \tag{2.17c}$$

The right side of Eq. (2.17a) is $O(1)$. However, the left side is $O(\varepsilon)$ because $X = O(1/\varepsilon)$. To ensure that Eq. (2.17a) is satisfied, we set the right side equal to zero, yielding:

$$-\frac{1}{3\overline{\Sigma}_t}\frac{d^2}{dz^2}\phi_0(z) + \overline{\sigma}_a\phi_0(z) = \overline{q} \quad . \tag{2.18}$$

Finally, we return to the original (unstretched) variables. Multiplying Eq. (2.18) by ε^2 and using:

$$\varepsilon^2\overline{\sigma}_a = p_1\varepsilon^2\sigma_{a1} + p_2\varepsilon^2\sigma_{a2} = p_1\Sigma_{a1} + p_2\Sigma_{a2} = \overline{\Sigma}_a \quad , \tag{2.19a}$$

$$\varepsilon^2\overline{q} = p_1\varepsilon^2 q_1 + p_2\varepsilon^2 q_2 = p_1 Q_1 + p_2 Q_2 = \overline{Q} \quad , \tag{2.19b}$$

$$\Phi_0(x) = \phi_0(\varepsilon x) = \phi_0(z) \quad , \tag{2.19c}$$

we obtain:

$$-\frac{1}{3\overline{\Sigma}_t}\frac{d^2}{dx^2}\Phi_0(x) + \overline{\Sigma}_a\Phi_0(x) = \overline{Q} \quad , \quad -X < x < X \quad . \tag{2.20}$$

Eq. (2.20) is the leading-order asymptotic limit of Eq. (2.7) as $\varepsilon \to 0$; it is also the conventional diffusion equation, with volume-averaged (atomic mix) cross sections. If the diffusion approximation were applied to the atomic mix transport equation that approximates Eq. (2.1), Eq. (2.20) would result. Thus, Eq. (2.20) contains the simplifications to Eq. (2.1) that come from both the atomic mix and diffusion approximations. We repeat that the above derivation shows that Eq. (2.20) is valid for problems in which optical widths of the material chunks are $O(1)$; for such problems, the atomic mix approximation has not previously been known to be valid.

Our asymptotic analysis does not yield boundary conditions for Eq. (2.20) that approximate the vacuum boundary conditions (2.1b) and (2.1c). In our numerical simulations, we used the extrapolated endpoint boundary conditions, taking the extrapolation distance to be twice the diffusion coefficient:

$$\Phi_0\left(X + \frac{2}{3\overline{\Sigma}_t}\right) = \Phi_0\left(-X - \frac{2}{3\overline{\Sigma}_t}\right) = 0 \quad . \tag{2.21}$$

These boundary conditions are heuristic, but we show that when used with Eq. (2.20), they very accurately predict the solution of Eqs. (2.1) in the diffusive atomic mix limit.

3. ASYMPTOTIC ANALYSIS OF THE LP EQUATIONS

To state the LP approximation to Eqs. (2.1), we must specify additional information [1,7-9]. For convenience, we assume that the system is *binary*, consisting of alternating chunks of two materials, labeled 1 and 2. The cross sections and source for material i ($i = 1$ or 2) are labeled Σ_i and Q_i. Also, we specify:

$$\lambda_i = \text{ the mean width of the chunks of material } i \quad , \tag{3.1a}$$

$$p_i = \frac{\lambda_i}{\lambda_1 + \lambda_2} = \text{ the volume fraction of material } i \quad . \tag{3.1b}$$

Then, the LP approximation to Eqs. (2.1) is:

$$\mu \frac{\partial \Psi_i}{\partial x}(x,\mu) + \Sigma_{ti}\Psi_i(x,\mu) = \frac{\Sigma_{si}}{2}\int_{-1}^{1} \Psi_i(x,\mu')d\mu' + |\mu| \left(\frac{\Psi_j(x,\mu)}{\lambda_j} - \frac{\Psi_i(x,\mu)}{\lambda_i} \right) + \frac{p_i Q_i}{2} \quad , \quad -X < x < X \ , \ -1 \le \mu \le 1 \ , \tag{3.2a}$$

$$\Psi_i(-X,\mu) = 0 \ , \ 0 < \mu \le 1 \ , \tag{3.2b}$$

$$\Psi_i(X,\mu) = 0 \ , \ -1 \le \mu < 0 \ . \tag{3.2c}$$

In these equations, $i = 1$ or 2 and $j = 2$ or 1, with $j \neq i$. [Thus, each of Eqs. (3.2) is really two equations.] After Eqs. (3.2) are solved, the LP estimate of $< \Psi >$, the mean angular flux – ensemble-averaged over all physical realizations – is:

$$< \Psi > (x,\mu) = \Psi_1(x,\mu) + \Psi_2(x,\mu) \ . \tag{3.2d}$$

The LP equations (3.2) are a simplification of Eqs. (2.1) because the cross sections in Eqs. (3.2a) are independent of x.

To analyze Eqs. (3.2) in the same asymptotic limit just applied to Eqs. (2.1), we take:

$$\Sigma_{ti} = O(1) \quad , \quad \lambda_i = O(1) \ , \tag{3.3a}$$

$$\Sigma_{ai} = \Sigma_{ti} - \Sigma_{si} = \varepsilon^2 \sigma_{ai} \quad , \quad Q_i = \varepsilon^2 q_i \ , \tag{3.3b}$$

$$z = \varepsilon x \quad , \quad X = O(1/\varepsilon) \ , \tag{3.3c}$$

$$\Psi_i(x,\mu) = \psi_i(z,\mu) \ . \tag{3.3d}$$

As before, the widths of the chunks are assumed to be comparable to a mean free path, x is scaled so that a chunk width and a mean free path are $O(1)$, absorption and sources are small [$O(\varepsilon^2)$], and – since there is no fast spatial variation in Eqs. (3.2) – the flux depends only on the slow spatial variable z and the angular variable μ. In his book [1], Pomraning considers an asymptotic diffusion approximation of Eqs. (3.2) in which the material chunks are optically thick. That asymptotic limit is fundamentally different from the asymptotic limit considered here. (Also, Pomraning does not apply a corresponding asymptotic limit to the original transport equation, so it is not known whether his result is physically correct.)

Introducing Eqs. (3.3) into (3.2), we obtain the scaled LP equations:

$$\varepsilon\mu \frac{\partial \psi_i}{\partial z}(z,\mu) + \Sigma_{ti}\psi_i(z,\mu) = \frac{\Sigma_{ti} - \varepsilon^2\sigma_{ai}}{2}\int_{-1}^{1} \psi_i(z,\mu')d\mu' + |\mu| \left(\frac{\psi_j(z,\mu)}{\lambda_j} - \frac{\psi_i(z,\mu)}{\lambda_i} \right) + \varepsilon^2 \frac{p_i q_i}{2} \ . \tag{3.4}$$

As before, we solve these equations by assuming the ansatz

$$\psi_i(z,\mu) = \sum_{n=0}^{\infty} \varepsilon^n \psi_{i,n}(z,\mu) \quad . \tag{3.5}$$

Introducing Eqs. (3.5) into (3.4) and equating the coefficients of different powers of ε, we obtain for $n \geq 0$,

$$\begin{aligned} &\Sigma_{ti}\left[\psi_{i,n}(z,\mu) - \frac{1}{2}\int_{-1}^{1}\psi_{i,n}(z,\mu')d\mu'\right] + |\mu|\left(\frac{\psi_{i,n}(z,\mu)}{\lambda_i} - \frac{\psi_{j,n}(z,\mu)}{\lambda_j}\right) \\ &\quad = -\mu\frac{\partial\psi_{i,n-1}}{\partial z}(z,\mu) - \frac{\sigma_{ai}}{2}\int_{-1}^{1}\psi_{i,n-2}(z,\mu')d\mu' + \delta_{n,2}\frac{p_i q_i}{2} \quad , \end{aligned} \tag{3.6}$$

where $\psi_{i,-1} = \psi_{i,-2} = 0$. Eqs. (3.6) can be solved recursively, first for $n = 0$, then $n = 1$, etc. The algebraic details are straightforward, so for brevity we will only state the important results here.

Eqs. (3.6) with $n = 0$ have only an isotropic solution of the form:

$$\psi_{i,0}(z,\mu) = \frac{p_i}{2}\phi_0(z) \quad , \tag{3.7}$$

where $\phi_0(z)$ is undetermined.

Eqs. (3.6) with $n = 1$ have a solvability condition, which is automatically satisfied. The general solution of the $n = 1$ equations is:

$$\psi_{i,1}(z,\mu) = \frac{p_i}{2}\left[\phi_1(z) - \mu f_i(|\mu|)\frac{d\phi_0}{dz}(z)\right] \quad , \tag{3.8}$$

where $\phi_1(z)$ is undetermined and:

$$f_i(|\mu|) = \frac{\lambda_1\lambda_2\Sigma_{tj} + (\lambda_1+\lambda_2)|\mu|}{\lambda_1\lambda_2\Sigma_{t1}\Sigma_{t2} + (\lambda_1\Sigma_{t1}+\lambda_2\Sigma_{t2})|\mu|} \quad . \tag{3.9}$$

Eqs. (3.6) with $n = 2$ have a solvability condition, which is not automatically satisfied. To obtain this condition, we (i) integrate Eqs. (3.6) with $n = 2$ over $-1 \leq \mu \leq 1$, and (ii) add the resulting two equations. This gives:

$$\begin{aligned} 0 = &-\frac{d}{dz}\int_{-1}^{1}\mu\left[\psi_{1,1}(z,\mu) + \psi_{2,1}(z,\mu)\right]d\mu \\ &-\int_{-1}^{1}\left[\sigma_{a1}\psi_{1,0}(z,\mu) + \sigma_{a2}\psi_{2,0}(z,\mu)\right]d\mu \\ &+ (p_1q_1 + p_2q_2) \quad . \end{aligned} \tag{3.10}$$

Introducing Eqs. (3.7) and (3.8) into Eq. (3.10) and simplifying, we obtain the following diffusion equation for ϕ_0:

$$-\frac{\gamma}{3\overline{\Sigma}_t}\frac{d^2\phi_0}{dz^2}(z) + \overline{\sigma}_a\phi_0(z) = \overline{q} \quad , \tag{3.11}$$

where

$$\overline{\sigma}_a = p_1\sigma_{a1} + p_2\sigma_{a2} \quad , \tag{3.12a}$$

$$\overline{q} = p_1q_1 + p_2q_2 \quad , \tag{3.12b}$$

$$\gamma = \int_0^1 3\mu^2\left(\frac{\mu+\alpha}{\mu+\beta}\right)d\mu \quad , \tag{3.12c}$$

$$\alpha = p_1^2\lambda_2\Sigma_{t2} + p_2^2\lambda_1\Sigma_{t1} \quad , \tag{3.12d}$$

$$\beta = \left[(\lambda_1\Sigma_{t1})^{-1} + (\lambda_2\Sigma_{t2})^{-1}\right]^{-1} \quad . \tag{3.12e}$$

Next, we return to the original (unscaled) variables. Multiplying Eq. (3.11) by ε^2 and using Eqs. (2.19), we obtain:

$$-\frac{\gamma}{3\overline{\Sigma}_t}\frac{d^2\Phi_0}{dx^2}(x)+\overline{\Sigma}_a\Phi_0(x)=\overline{Q}\ \ ,\ \ -X<x<X\ \ . \tag{3.13}$$

Finally, Eqs. (3.2d), (3.3d), (3.5), (3.7), (3.1b), and (2.19) give:

$$\begin{aligned}\Phi(x)&=\int_{-1}^{1}\Psi(x,\mu)d\mu\\&=\int_{-1}^{1}\left[\Psi_1(x,\mu)+\Psi_2(x,\mu)\right]d\mu\\&=\int_{-1}^{1}\left[\psi_1(z,\mu)+\psi_2(z,\mu)\right]d\mu\\&=p_1\phi_0(z)+p_2\phi_0(z)+O(\varepsilon)\\&=\phi_0(z)+O(\varepsilon)\\&=\Phi_0(x)+O(\varepsilon)\ \ .\end{aligned} \tag{3.14}$$

Thus, Eq. (3.13) is the leading-order asymptotic limit of Eq. (3.4) as $\varepsilon\to 0$, and the unknown $\Phi_0(x)$ in this equation is the leading-order estimate of the scalar flux.

Our asymptotic analysis does not yield "vacuum" boundary conditions for Eq. (3.13). In our numerical simulations, we used the extrapolated endpoint boundary conditions, as before taking the extrapolation distance to be twice the diffusion coefficient:

$$\Phi_0\left(X+\frac{2\gamma}{3\overline{\Sigma}_t}\right)=\Phi_0\left(-X-\frac{2\gamma}{3\overline{\Sigma}_t}\right)=0\ \ . \tag{3.15}$$

These boundary conditions are heuristic, but we show that when used with Eq. (3.13), they very accurately predict the solution of Eqs. (3.2) in the diffusive atomic mix limit.

We note that because of the presence of the constant γ, Eq. (3.13) is not the correct atomic mix diffusion equation. In fact, the easily-obtained identity

$$\alpha-\beta=\left(\frac{\lambda_1\lambda_2}{\lambda_1+\lambda_2}\right)^2\frac{(\Sigma_{t2}-\Sigma_{t1})^2}{\lambda_1\Sigma_{t1}+\lambda_2\Sigma_{t2}} \tag{3.16}$$

shows that if $\Sigma_{t2}\neq\Sigma_{t1}$, then $\alpha>\beta$, and hence by Eq. (3.12c), $\gamma>1$. In this case, for any choice of λ_1 and λ_2, the diffusion coefficient in Eq. (3.13) is unphysically large. This has the effect of incorrectly "flattening" the solution of Eq. (3.13) in comparison to the correct atomic mix diffusion solution. Eq. (3.16) also shows that as $\lambda_i\to 0$, $\alpha\to\beta$, so $\gamma\to 1$. Thus, if the chunk widths become small, the LP diffusion solution does correctly limit to the atomic mix diffusion result.

4. NUMERICAL RESULTS

To test the predictions of the asymptotic analysis, we first consider Eq. (2.1) for spatially periodic systems consisting of M cells, each of width $\ell=\ell_1+\ell_2$, defined by:

$$\Sigma_t(x)=\begin{cases}\Sigma_{t1} & 0<x<\ell_1\\ \Sigma_{t2} & \ell_1<x<\ell\end{cases}\ \ ,$$

$$\Sigma_a(x) = \begin{cases} \frac{\sigma_{a1}}{M^2} & 0 < x < \ell_1 \\ \frac{\sigma_{a2}}{M^2} & \ell_1 < x < \ell \end{cases} , \tag{4.1a}$$

$$Q(x) = \begin{cases} \frac{q_1}{M^2} & 0 < x < \ell_1 \\ \frac{q_2}{M^2} & \ell_1 < x < \ell \end{cases} . \tag{4.1b}$$

These functions are extended periodically across the full system $-X \leq x \leq X = M\ell/2$, and vacuum boundary conditions are assigned at the outer boundaries $x = \pm X$. [Here, Σ_{tn}, σ_{an}, and q_n are $O(1)$ constants; $M >> 1$, and $\varepsilon = 1/M$.] For each M, the atomic mix approximation to Eq. (2.1a) contains the following volume-averaged cross sections and source:

$$\overline{\Sigma}_t = \frac{\Sigma_{t1}\ell_1 + \Sigma_{t2}\ell_2}{\ell} \quad , \quad \overline{\Sigma}_a = \frac{\sigma_{a1}\ell_1 + \sigma_{a2}\ell_2}{M^2\ell} \quad , \quad \overline{Q} = \frac{q_1\ell_1 + q_2\ell_2}{M^2\ell} \ , \tag{4.2}$$

and the system half-width is again $X = M\ell/2$.

We specifically consider problems of the above form with M = 10, 20, and 40, and:

n	ℓ_n	Σ_{tn}	σ_{an}	q_n
1	3.0	1.0	0.1	0.2
2	3.0	0.0	0.0	0.0

In these problems, the spatial cells are 3.0 mean free paths thick; they are *not* optically thin. Also, material 1 is highly-scattering and material 2 is a void. [Material 2 being a void does not violate any of our physical assumptions, it corresponds to well-known physical applications (e.g. pebble-bed reactors cores), and it leads to significant discrepancies in the LP predictions.]

Our numerical results, plotted in Figure 1, were generated using the LTS_N method [11] to solve the heterogeneous-medium transport Eq. (2.1), the atomic mix approximation to Eq. (2.1), and the LP approximation (3.2). These simulations produced, respectively, the Exact Scalar Flux, the Atomic Mix Scalar Flux, and the Exact LP Scalar Flux plotted in the figure. The Atomic Mix Diffusion Scalar Flux and LP Diffusion Scalar Flux, also plotted in the figure, were obtained by analytically solving Eqs. (2.20) and (2.21), and (3.13) and (3.15).

The three plots in Figure 1, corresponding to $\varepsilon = 1/M = 0.1, 0.05,$ and 0.025, show that the exact scalar flux, the atomic mix scalar flux, and the atomic mix diffusion scalar flux increasingly agree as M increases (ε decreases). Also, the exact LP scalar flux significantly disagrees with these results in a way that is accurately predicted by the theory.

We have also considered "random" versions of the above "periodic" problems. In the "random" problems, all of the parameters defined above (including the width of the systems) are still used – except that the widths of the individual material chunks are sampled from an exponential distribution with the mean values ℓ_1 and ℓ_2 specified above. Thus, the systems have specified widths but are no longer periodic; they consist of many layers of random thicknesses. (The LP approximation was developed to model precisely this type of problem.) To simulate these random systems, for each M we generated 10,000 different realizations, solved Eqs. (2.1) for each realization, and averaged the scalar fluxes to obtain the ensemble-averaged scalar fluxes. The results are plotted in Figure 2. As in Figure 1, these plots show that: (i) the Ensemble-Averaged Scalar Flux, the Atomic Mix Scalar Flux, and the Atomic Mix Diffusion Scalar Flux agree, and (ii) the Exact LP Scalar Flux has a systematic error that is accurately predicted by the asymptotic theory.

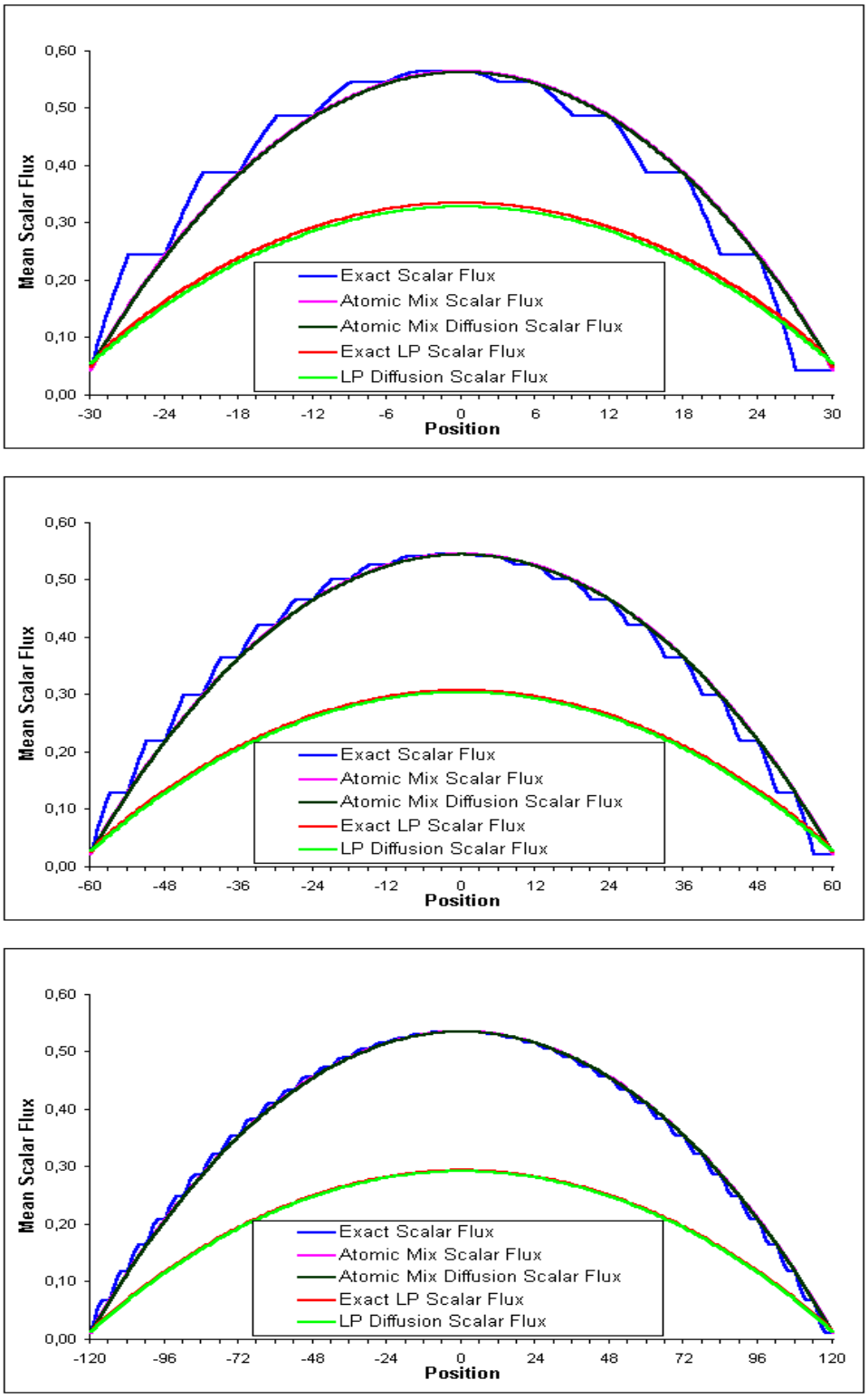

Figure 1: The "Periodic" Problem: M=10 (Top), M=20 (Middle), and $M = 40$ (Bottom)

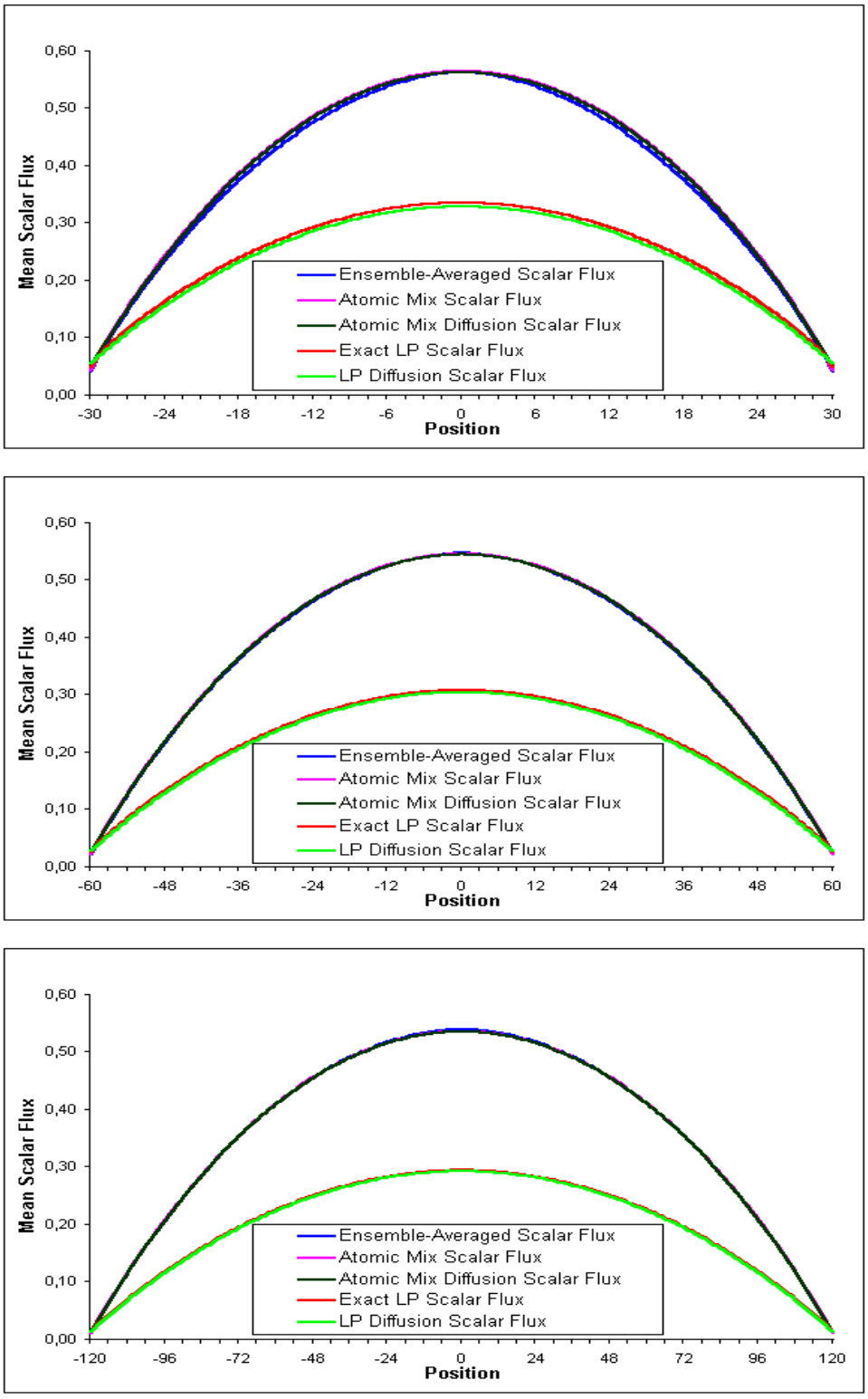

Figure 2: The "Random" Problem: M=10 (Top), M=20 (Middle), and $M = 40$ (Bottom)

5. DISCUSSION

The asymptotic analysis developed in this paper shows that under certain *diffusive* conditions, the atomic mix approximation to the transport equation is valid for 1-D heterogeneous-medium problems in which the individual layers ("chunks") of materials are not optically thin. Specifically: the physical system should (i) have weak absorption and sources, (ii) be optically thick, and (iii) consist of a large number of material layers, whose thicknesses are comparable to (or small compared to) a mean free path. It is not necessary that the system be highly-scattering at all points; void regions are permitted. A related asymptotic analysis, applied to the LP equations, shows that the LP model deviates from the correct (atomic mix diffusion) result in a way that is confirmed by our numerical results. This provides a theoretical explanation for the previously-observed inaccuracies in the LP model for diffusive problems.

The asymptotic limit considered in this paper is one for which the leading-order flux depends only on "volume-averaged" data; fluctuations from this result are small. Therefore, the analysis applies to either (i) a specific problem, in which the detailed space-dependence of the cross sections is known, or (ii) a "random" problem, in which only volume-averaged cross sections are known, and an estimate of the ensemble-averaged flux is desired. In both cases, the fluctuation from the atomic mix diffusion prediction is small. It is possible that the asymptotic analysis can be generalized, in ways that would require minimal extra geometrical information, to provide useful bounds on these small fluctuations.

Also, the results developed in this paper can be extended to multidimensional problems, but the relatively simple "diffusive atomic mix" result derived here no longer generally holds. For example, 3-D transport in the 1-D physical systems treated in this paper leads to an anisotropic diffusion equation of the form

$$-\frac{1}{3\overline{\Sigma}_t}\frac{\partial^2}{\partial x^2}\Phi_0(x,y,z) - D_\perp\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Phi_0(x,y,z) + \overline{\Sigma}_a\Phi_0(x,y,z) = \overline{Q} \ , \tag{5.1}$$

where $D_\perp \neq 1/3\overline{\Sigma}_t$. The diffusion coefficient in the y and z-directions differs from the diffusion coefficient in the x-direction because the spatial heterogeneities are correlated: if a point at depth $x = x_0$ is in material i, then all points (x_0, y, z) at the same depth are also in material i. For more general 3-D problems, any spatial correlations of the cross sections can also lead to anisotropic diffusion.

In future work, we hope to extend the asymptotic analysis developed in this paper to these and other more realistic problems. In addition, this asymptotic analysis provides a theoretical tool for examining future generalizations of the LP model, which might – for example – be aimed at correcting the deficiency described above.

ACKNOWLEDGMENTS

M.T. Vilhena is gratefully indebted to CNPq for partial financial support.

REFERENCES

1. G.C. Pomraning, *Linear Kinetic Theory and Particle Transport in Stochastic Mixtures*, World Scientific Press, Singapore (1991).

2. L. Dumas and F. Golse, "Homogenization of Transport Equations," *SIAM J. Appl. Math.* **60**, 1447 (2000).

3. G.J. Habetler and B.J. Matkowsky, "Uniform Asymptotic Expansions in Transport Theory with Small Mean Free Paths, and the Diffusion Approximation," *J. Math. Phys.* **16**, 846 (1975).

4. E.W. Larsen and J.B. Keller, "Asymptotic Solution of Neutron Transport Problems for Small Mean Free Paths," *J. Math. Phys.* **15**, 75 (1974).

5. E.W. Larsen, "Diffusion Theory as an Asymptotic Limit of Transport Theory for Nearly Critical Systems with Small Mean Free Paths," *Ann. Nucl. Energy* **7**, 249 (1980).

6. E.W. Larsen, "Asymptotic Derivation of the Atomic-Mix Diffusion Model for 1-D Random Media," *Trans. Am. Nucl. Soc.* **89**, 296 (2003).

7. G.C. Pomraning, "Transport in Discrete Stochastic Mixtures," *Transport Theory Statist. Phys.* **27** 405 (1998).

8. G.C. Pomraning, "Radiative Transfer and Transport Phenomena in Stochastic Media," *Int. J. Eng. Sci.* **36**, 1595 (1998).

9. A. Davis and A. Marshak (editors), *3-D Radiative Transfer in the Atmosphere (Physics of Earth and Space Environments)*, Springer (2005).

10. I.M. Davis, T.S. Palmer, and E.W. Larsen, "A Comparison of Binary Stochastic Media Transport Models in 'Solid-Void' Mixtures," *Proc. PHYSOR 2004 – The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments*, Chicago, Illinois, April 25-29, 2004, American Nuclear Society, Lagrange Park, IL (2004).

11. C.F. Segatto and M.T. Vilhena, "The State of Art of the LTS_N Method," Proc. ANS Topical Meeting: *Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications*, September 27-30, 1999, Madrid, **2**, 1618 (1999).