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A CRITIQUE OF THE MODIFIED LEVERMORE-POMRANING MODEL

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ABSTRACT

The Levermore-Pomraning and modified Levermore-Pomraning models are compared using theoretical considerations. Numerical results for these models are presented for a set of standard tests in finite slabs as well as for related problems.

Key Words: linear transport, stochastic media.

1 INTRODUCTION

Transport in stochastic materials has applications in radiative transfer as well as reactor analysis. The relevant quantities of interest are the so-called material fluxes. These are the ensemble averaged fluxes for the set of physical realizations that have a given material in the same geometrical location. A system of exact transport-like coupled equations for the material fluxes was independently derived by Adams et al. (1989) and by Sanchez (1989), but these equations are not closed. Correlation terms appear that depend on new ensemble averaged fluxes, called interface fluxes. These new fluxes are the averages over the realizations that have one material to the left of a geometrical location and a different material to the right of the location, along a given direction of particle motion. When the material chord lengths follow Markov statistics and the materials are purely absorbing one finds that the transition flux equals the material flux for the upstream material. This natural closure has been invoked to derive a set of closed equations for the general case of transport with collisions. These equations are known as the Levermore-Pomraning (LP) model (Levermore et al.,1988;Pomraning,1991) and can be applied to a multidimensional geometry. For the purpose of this paper we need only the one-dimensional slab form for a bimaterial stochastic mixture:

$$\begin{aligned}
(\mu\partial_x + \Sigma_k) < \psi_k > = H_k < \psi_k > + S_k + |\mu| \tfrac{p_{k'}}{p_k \lambda_{k'}} (< \psi_{k'} > - < \psi_k >), \qquad & x_L < x < x_R, \\
< \psi_k > = \psi_k^L(\mathbf{v}), \qquad & x = x_L,\ 0 < \mu < 1, \\
< \psi_k > = \psi_k^R(\mathbf{v}), \qquad & x = x_R,\ -1 < \mu < 0.
\end{aligned}$$

Here $k = 1, 2$ denotes one of the materials and $k' = 3 - k$. The $\Sigma_k(x)$, $H_k(x)$ and $S_k(x, \mathbf{v})$ are the total cross section, the scattering operator and the source for material k, λ_k and p_k are the mean chord length and the probability for material k at position x, respectively, and, with $\mathbf{v} = (\mu, E)$, the $< \psi_k > (x, \mathbf{v})$ are the material fluxes, obtained by ensemble averaging of the flux over the realizations that have material k at location x.

Recently, Akcasu has proposed a modification of the LP model. The modified MLP equations (Akcasu,2006) have the advantage of given exact results for a special half space problem as well as for related full space problems. They have also proved to give the atomic mix diffusion equation at the diffusive limit, even for finite chord lengths (Larsen,2006). Although the model has been analyzed for use in finite rod problems, at present time there is not a clear consensus as to how apply the MLP equations for more realistic finite-slab problems. The aim of this work is to analyze the straightforward application of the MLP equations to finite slab problems and to present a numerical comparison between LP and MLP for a set of standard problems (Zuchuat et al.,1994) as well as for related source problems. We stress that in our approach we use MLP with the natural boundary conditions of the problem.

In the next section we follow the early work by Pomraning (Pomraning,1991) to define the special class of half space problems for which one can obtain exact results for the ensemble average flux for bimaterial Markovian statistics. In the following section we use the formalism established by Pomraning, based on the probability $P_k(\tau;x)d\tau$ for a realization to have $\tau(x,\omega)\in(\tau,\tau+d\tau)$ and $\omega(x)=k$, to derive Akcasu's MLP equations. In Section 4 we give a comparative analysis of the LP and MLP models based on already established and new theoretical results. Numerical results are presented in Section 5 and conclusions are given in the last section. Related material has been relegated to the appendices. A short derivation of the Master equation for the $P_k(\tau;x)$ is given in Appendix A. In Appendix B we explore the construction of the propagator used by Akcasu (Akcasu,2006). Finally, in Appendix C we discuss a stable numerical algorithm for the solution of the MLP model.

2 A RESTRICTED EXACT TREATMENT

We consider linear particle transport in a half-space slab geometry comprising a random material. We denote by $\Omega=\{\omega,p(\omega)\}$ the space of all physical realizations with $p(\omega)\geq 0$ and $\int_\Omega p(\omega)d\omega=1$. Every realization $\omega\in\Omega$ consists of a triplet of functions $\omega\rightarrow(\Sigma_\omega,\Sigma_{s,\omega},S_\omega)$, where, with $\mathbf{v}=(\mu,E)$, $\Sigma_\omega(x,\mathbf{v})$ and $\Sigma_{s,\omega}(x,\mathbf{v}'\rightarrow\mathbf{v})$ are the total and differential scattering cross sections and $S_\omega(x,\mathbf{v})$ is the external source. Therefore, the flux $\psi_\omega(x,\mathbf{v})$ satisfies the equation:

$$\begin{array}{cc}(\mu\partial_x+\Sigma_\omega)\psi_\omega=H_\omega\psi_\omega+S_\omega, & x_L<x<\infty,\\ \psi_\omega(x,\mathbf{v})=\psi_L(\mathbf{v}), & x=x_L,\ \mu>0,\\ \psi_\omega(x,\mathbf{v})<\infty, & x\rightarrow\infty,\end{array}\tag{1}$$

where H_ω is the scattering operator

$$(H_\omega\psi_\omega)(x,\mathbf{v})=\int d\mathbf{v}'\Sigma_{s,\omega}(x,\mathbf{v}'\rightarrow\mathbf{v})\psi_\omega(x,\mathbf{v}').$$

In order to establish exact results in the presence of scattering, Pomraning introduced a 'restricted exact treatment' (Pomraning,1991) by considering a homogeneous material with stochastic density such that the material properties $(\Sigma_\omega,\Sigma_{s,\omega},S_\omega)$ have the same spatial dependence:

$$\begin{array}{c}\Sigma_\omega(x,\mathbf{v})=N_\omega(x)\sigma(\mathbf{v}),\\ \Sigma_{s,\omega}(x,\mathbf{v}'\rightarrow\mathbf{v})=N_\omega(x)\sigma_s(\mathbf{v}'\rightarrow\mathbf{v}),\\ S_\omega(x,\mathbf{v})=N_\omega(x)s(\mathbf{v}),\end{array}$$

where $N_\omega(x)$ is the stochastic density for the realization ω, that now consists of a single function $\omega\rightarrow(N_\omega)$, with $\sigma(\mathbf{v})>0$ and $\sigma_s(\mathbf{v}'\rightarrow\mathbf{v})$, $s(\mathbf{v})\geq 0$ common to all realizations in Ω.

By introducing the density ('optical') thickness

$$\tau(x,\omega) = \int_{x_L}^{x} N_\omega(y)dy \tag{2}$$

and, by changing variables $x \rightarrow \tau(x,\omega)$ so that $\partial_x \rightarrow (\partial_x \tau)\partial_\tau = N_\omega(x)\partial_\tau$, one can write (1) in terms of the flux $\widehat{\psi}(\tau,\mathbf{v}) = \psi_\omega(x,\mathbf{v})$:

$$\begin{array}{cc} (\mu\partial_\tau + \sigma)\widehat{\psi} = h\widehat{\psi} + s, & 0 < \tau < \infty, \\ \widehat{\psi}(\tau,\mathbf{v}) = \psi_L(\mathbf{v}), & \tau = 0,\ \mu > 0, \\ \widehat{\psi}(\tau,\mathbf{v}) < \infty, & \tau \rightarrow \infty, \end{array} \tag{3}$$

where scattering operator h is like H but with kernel $\sigma_s(\mathbf{v}' \rightarrow \mathbf{v})$.

Note that the deterministic flux $\widehat{\psi}(\tau,\mathbf{v})$ is the same for all realizations. Following Pomraning (1991) we define the density of probability $P(\tau;x)$, such that $P(\tau;x)d\tau$ is the probability for a realization ω to have $\tau(x,\omega) \in (\tau, \tau + d\tau)$. Then, the ensemble average flux at position x can be written as

$$< \psi(x,\mathbf{v}) >= \int_\Omega \psi_\omega(x,\mathbf{v})p(\omega)d\omega = \int_0^\infty \widehat{\psi}(\tau,\mathbf{v})P(\tau;x)d\tau. \tag{4}$$

The above result applies to a half space (HS) comprising a homogeneous material with stochastic density (SD) and with deterministic incoming angular flux and a deterministic external source. We shall refer to this problem as the HSSD problem. As an aside comment we observe that $P(\tau;0) = \delta(\tau)$ and that, therefore, the ensemble average of the exiting angular flux for the HSSD problem is deterministic, $< \psi(0,\mathbf{v}) >= \widehat{\psi}(0,\mathbf{v})$, hence, independent of the statistical set (Pomraning,1991). Furthermore, a deeper result is obtained from $\psi_\omega(0,\mathbf{v}) = \widehat{\psi}(0,\mathbf{v})$ which shows that the boundary fluxes are the same for each realization. Notice that this property is necessary to prove that (ψ_ω,ω) is a joint Markovian process, a necessary condition for the derivation of the MLP equations from the jump probabilities associated to this process (Van Kampen,1992).

Pomraning considered a statistical set of binary homogeneous Markov realizations with material probabilities p_k ($k = 1,2$) and introduced the conditional probabilities $f_k(\tau;x)d\tau$ = probability for $\tau(x,\omega) \in (\tau, \tau + d\tau)$ given that x lies in material k. Pomraning also derived analytical expressions for the $f_k(\tau;x)$. Hence, by replacing $P(\tau;x) = \sum_{k=1}^2 p_k f_k(\tau;x)$ in Eq. (4) and by using the analytical expressions for the $f_k(\tau;x)$ one obtains an *explicit* formula to compute the ensemble average flux. Pomraning used this approach to analyze a number of half and full space problems (Pomraning,1991).

In this work, we depart from Pomraning's approach and follow Akcasu (2006) to derive an *implicit* formula for the ensemble average flux in the form of transport-like equations for the material fluxes. For bimaterial statistics we write $P(\tau;x) = \sum_{k=1}^2 P_k(\tau;x)$, where $P_k(\tau;x)d\tau$ is the probability for $\tau(x,\omega) \in (\tau, \tau + d\tau)$ and $\omega(x) = k$ so that $N_\omega(x) = N_k(x)$. We have then

$$< \psi(x,\mathbf{v}) >= \sum_{k=1}^{2} \psi_k(x,\mathbf{v}),$$

where, with $\Omega_k(x) = \{\omega \in \Omega, \omega(x) = k\}$ denoting the set of realizations that have material k at x,

$$\psi_k(x,\mathbf{v}) = \int_{\Omega_k(x)} \psi_\omega(x,\mathbf{v})p(\omega)d\omega = \int_0^\infty \widehat{\psi}(\tau,\mathbf{v})P_k(\tau;x)d\tau. \tag{5}$$

The basic idea to derive transport-like equations for the $\psi_k(x,\mathbf{v})$ is to differentiate (5) with respect to x to obtain

$$(\partial_x\psi_k)(x,\mathbf{v}) = \int_0^\infty \widehat{\psi}(\tau,\mathbf{v})(\partial_x P_k)(\tau;x)d\tau \tag{6}$$

and to introduce a dynamic equation for $\partial_x P_k$. As we show in the next section, such a dynamic equation can be written down when the bimaterial statistics are Markovian. Another possibility would be to compute the $\partial_x P_k$ from the analytical expressions obtained by Pomraning for the $f_k(\tau;x)$ for the case of stationary bimaterial Markov statistics.

3 DERIVATION OF THE MLP EQUATIONS

We consider a statistical set of realizations with bimaterial Markovian chord distributions. Each material is characterized by a bounded deterministic density $N_k(x)$ ($k=1,2$) and each realization ω is a binary Markov process with $\omega(x)\in\{1,2\}$ that assigns material $k=\omega(x)$ to position x. We consider the general case of inhomogeneous statistics and denote by $1/\lambda_k(x)$ the transition probability per unit length from material k into material $k'=3-k$. We observe that the density distance (2) obeys the stochastic differential equation

$$(\partial_x\tau)(x,\omega) = N_\omega(x)$$

with a deterministic initial condition $\tau(x_L,\omega)=0$. Therefore the pair (τ,ω) defines a Markov process and this allows to obtain a dynamic equation for the $\partial_x P_k$. Here we use the general formulation established by Van Kampen (1992) to directly write down the master equation for the P_k,

$$\partial_x P_k = -\partial_\tau(N_\omega P_k) + P_{k'}/\lambda_{k'} - P_k/\lambda_k, \tag{7}$$

while in Appendix A we give a straightforward derivation of this formula. Next, we replace (7) in (6) to obtain

$$(\mu\partial_x + \Sigma_k)\psi_k = H_k\psi_k + p_k S_k + \mu(\psi_{k'}/\lambda_{k'} - \psi_k/\lambda_k), \tag{8}$$

subject to the boundary conditions

$$\begin{array}{cc} \psi_k(x,\mathbf{v}) = p_k(x_L)\psi_L(\mathbf{v}), & x=x_L,\ \mu>0, \\ \psi_k(x,\mathbf{v})<\infty, & x\to\infty. \end{array} \tag{9}$$

To derive the MLP equations in (8,9) we have carried out an integration by parts for the integral $\int_0^\infty \widehat{\psi}(\tau,\mathbf{v})\times \partial_\tau(N_\omega P_k)d\tau$ and used Eq. (3) in the result. Note that the boundary term $\widehat{\psi}\partial_\tau(N_\omega P_k)\Big|_0^\infty$ cancels out because $\widehat{\psi}$ is bounded and $P_k(0;x)=P_k(\infty;x)=0$ for $x\in(x_L,\infty)$.

Finally, in boundary conditions (9),

$$p_k(x) = \int_{\Omega_k(x)} p(\omega)d\omega = \int_0^\infty P_k(\tau;x)d\tau$$

is the probability for material k at x. The dynamics for the p_k are straightforwardly obtained by integrating (7) over τ:

$$\partial_x p_k = p_{k'}/\lambda_{k'} - p_k/\lambda_k \tag{10}$$

with given initial values $p_k(x_L)$ satisfying $p_k(x_L)+p_{k'}(x_L)=1$. Note that the values $p_k(x_L)$ uniquely define the set of Markovian realizations Ω.

4 ANALYSIS OF THE MLP MODEL

Akcasu (2006) analyzed the boundary conditions to be used with the MLP model for a finite slab and introduced a stochastic propagator to propose a possible application of the MLP equations (8) for finite slabs. These equations have the advantage of given the exact solution with scattering for the HSSD problem. In this section we compare the MLP with natural boundary conditions and the LP models, while in the next section we present a numerical comparison for some finite-slab problems.

4.1 The purely absorbing limit

The first point we shall discuss is the limiting case when there is no scattering. As it is well known, the LP model is exact in this limit for Markovian chord statistics. Hence, one would expect that the LP solution for a small scattering perturbation around this limit case will give accurate results, while probably this will not be the case for the MLP model, which does not have the correct form at the zero-scattering limit. However, this raises the question of why the MLP model is correct for the HSSD problem with no scattering. The answer, as we will show, is that in this case the ensemble average fluxes $< \psi_k(x, \mathbf{v}) >= \psi_k(x, \mathbf{v})/p_k(x)$ for negative μ's are constant and, therefore, independent of k, and this makes the correlation terms in Eqs. (8) to cancel one each other. This is best viewed by writing (8) for the ensemble average fluxes:

$$(\mu\partial_x + \Sigma_k) < \psi_k >= H_k < \psi_k > +S_k + \mu\frac{p_{k'}}{p_k\lambda_{k'}}(< \psi_{k'} > - < \psi_k >), \tag{11}$$

where the last term on the right-hand-side contains the correlation contribution. For the purely absorbing case and for $\mu < 0$ the exact correlation term, as predicted by LP theory, has a minus sign. Thus, for the MLP formulation to be right one must have $< \psi_{k'} >=< \psi_k >$ for $\mu < 0$.

Indeed, consider these equations for the HSSD problem without scattering. Note that the solution of Eq. (3) for no scattering and $\mu < 0$ is

$$\widehat{\psi}(\tau, \mathbf{v}) = \int_0^\infty e^{-\sigma(\mathbf{v})z} s(\mathbf{v}) dz = s(\mathbf{v})/\sigma(\mathbf{v}),\ \mu < 0,$$

that, in view of (5), results in $< \psi_k(x, \mathbf{v}) >= s(\mathbf{v})/\sigma(\mathbf{v}),\ \mu < 0$. It is easily verified that this is the solution of (11) for $\mu < 0$.

Another way to see this result is to note that for negative μ the fluxes at position x can be obtained from a 'modified' HSSD problem for the half space with left boundary $x > x_L$ that we describe with the spatial variable y, $0 < y < \infty$. This new HSSD problem has as boundary values for the $p_k(y = 0)$ the $p_k(x)$ values obtained from Eqs. (10). Next, we use the fact that the exiting boundary fluxes for the HSSD problem are deterministic so that for the modified HSSD problem, with $\tau = 0$ at position $y = 0$, we have $P_k(\tau; 0) = p_k(x)\delta(\tau)$ and we can write

$$\psi_k(x, \mathbf{v}) = p_k(x)\widehat{\psi}(0, \mathbf{v}) \rightarrow < \psi_k(x, \mathbf{v}) >= \widehat{\psi}(0, \mathbf{v}),\ \mu < 0.$$

We conclude that for the purely absorbing HSSD problem the MLP equations are correct because the correlation terms vanish for $\mu < 0$. A property that results from the particular combination of random density bimaterial statistics and a half-space geometry (for which the exiting directions have infinite-length trajectories.)

4.2 Relaxation lengths for the spatial modes

Another property that has been claimed for the MLP model is that this model can yield the correct relaxation lengths for the spatial modes (Akcasu,2007a). This prediction is based on writing the solution for a final slab with left and right entering fluxes, $\psi^L_{in}(\mathbf{v})$ and $\psi^R_{in}(\mathbf{v})$, and zero internal sources as

$$\psi_\omega(x,\mathbf{v}) = (U_\omega \psi^L_\omega)(x,\mathbf{v}), \tag{12}$$

where $\psi^L_\omega(\mathbf{v}) = \psi_\omega(x_L,\mathbf{v})$ are the boundary fluxes at the left for all μ directions and $U_\omega(x,\mathbf{v})$ is a linear operator satisfying

$$(\mu\partial_x + \Sigma_\omega)U_\omega = H_\omega U_\omega$$

with the left boundary condition $U_\omega(x_L,\mathbf{v}) = 1$ for $\forall\mu$. To complete formulation (12) one has to express the exiting left flux in terms of the right entering flux. But this makes the boundary term dependant on operator U_ω and, therefore, stochastic. Following Akcasu (2006), the MLP model could be used to exactly compute the average $< U(x,\mathbf{v}) >$ and, therefore, an approximation for the flux could be obtained from the expression

$$< \psi(x,\mathbf{v}) > \sim < U(x,\mathbf{v}) >< \psi^L(x_L,\mathbf{v}) >, \tag{13}$$

where the ensemble average of $< \psi^L(x_L,\mathbf{v}) >$ is computed by using the exact average $< U(x,\mathbf{v}) >$. Akcasu concludes that this solution correctly predicts the exact relaxation modes because $< U(x,\mathbf{v}) >$ can be calculated exactly with the MLP model. This conclusion seems contradictory with the fact that the MLP model is only exact for the HSSD problem. Calculation of the exact ensemble average of $U(x,\mathbf{v})$ in a finite slab involves a problem with two stochastic parameters $\tau(x,\omega)$ and $\tau(x_R,\omega)$ and therefore depends on the probability $P(\tau,\tau_R;x)d\tau d\tau_R$ for a realization $\omega\in\Omega$ to have $\tau(x,\omega)\in(\tau,\tau+d\tau)$ and $\tau(x_R,\omega)\in(\tau_R,\tau_R+d\tau_R)$ (Pomraning,1991). Equivalently, as shown in Appendix B, construction of $U(x,\mathbf{v})$ requires knowing the Green's functions and therefore the exact transport solutions for the finite slab.

Nevertheless, use of (13) for a finite slab preserves the infinite-medium (diffusion) modes, while LP does not. But only an exact model for a finite slab will preserve the modes that are actually excited by the natural boundary conditions of the problem.

4.3 The diffusion limit

An extensive analysis of the behavior of the Levermore-Pomraning (LP) model in the diffusion limit was presented in (Malvagi et al.,1992). The authors took stock of the diffusion limit of the transport equation with the scaling

$$\Sigma \sim O(1), \mu\partial_x \sim O(\epsilon), \Sigma_a, S \sim O(\epsilon^2)$$

and considered a variable scaling for the Markovian transition probabilities $1/\lambda_k \sim O(\epsilon^n)$. They found four different behaviors: weak coupling ($n \geq 3$), moderate coupling ($n = 1$), strong coupling ($n = 0$) and atomic mix ($n \leq -1$). The result shows that both, strong coupling and atomic mix, yield an asymptotic diffusion equation for the homogeneous mixture. However, while atomic mix predicts the expected diffusion coefficient, $D = 1/(3 < \Sigma >)$, for strong coupling one finds a different diffusion coefficient, which depends on the Σ_k and the λ_k values (Malvagi et al.,1992).

Recently, Larsen et al. (Larsen et al.,2005) revisited the diffusion limit for the LP model for the case of strong coupling and atomic mix ($n \leq 0$) and found the same results as in the previous study by Malvagi et al. However, Larsen et al. analyzed also the diffusion limit of the transport equation for a deterministic

medium composed of alternate lamps of materials with widths l_k. For strong coupling , $l_k\Sigma_k \sim O(1)$, they found the transport equation limits to the diffusion equation with the familiar diffusion coefficient $D = 1/(3\overline{\Sigma})$, where $\overline{\Sigma}$ is the total cross section of the homogenized material:

$$-\partial_x \frac{1}{3\overline{\Sigma}} \partial_x \Phi + \overline{\Sigma}_a \Phi + \overline{Q} = 0. \tag{14}$$

Because this result applies to most of the realizations one concludes that the ensemble average flux obeys (14) with the ensemble averaged cross sections and sources. The analysis was confirmed by numerical experiments that showed that for strong coupling, $\lambda_k\Sigma_k \sim O(1)$, binary Markovian statistics limits to the classical diffusion equation, while LP and its diffusion limit yield a different result (Larsen et al.,2005). Lately, Larsen analyzed the MLP equations (Larsen,2006) in the diffusion limit with strong coupling and found that MLP limits to the diffusion equation with the ensemble averaged diffusion coefficient $D = 1/(3 < \Sigma >)$ predicted by atomic mix limit; this contrasts with the result previously obtained for the LP model (Malvagi et al.,1992;Larsen et al.,2005). The conclusion is that the MLP equations are also exact (while LP is not) at the diffusion limit with strong coupling (Larsen.,2006).

4.4 Left boundary condition

Because of the unusual sign of the correlation term for negative μ values, there is a doubt as to whether the MLP model should be only used with zero right incoming flux for finite slabs. To see that this should not always be the case, consider the two following problems:

(A) The HSSD problem in (x_L, ∞).

(B) A finite slab problem obtained by restricting every realization of problem A to (x_L, x_R) and by adding the appropriate right boundary condition: $(\psi_\omega)_B(x_R, \mathbf{v}) = (\psi_\omega)_A(x_R, \mathbf{v})$ for $\mu < 0$..

Clearly, these two problems have the same material fluxes $\psi_k(x, \mathbf{v})$ in (x_L, x_R). Moreover, the MLP equations for problem B give the exact values for the (x_L, x_R) if one uses as right boundary condition

$$(\psi_k)_B(x_R, \mathbf{v}) = (\psi_k)_A(x_R, \mathbf{v}), \quad \mu < 0, \tag{15}$$

where $(\psi_k)_A(x_R, \mathbf{v})$ are the exact material fluxes (as given, by example, by the MLP equations for problem A). Notice that this boundary condition is not deterministic.

We conclude that for this finite-slab problem the MLP is exact if one uses as right boundary condition the non-zero fluxes in (15).

4.5 Symmetry

Consider a finite slab for $x \in (-a, a)$ with symmetric boundary conditions, $\psi_{in}(-a, \mathbf{v}) = \psi_{in}(a, -\mathbf{v})$ for $\mu > 0$, comprising a homogeneous, symmetrical bimaterial Markovian mixture with constant material properties. Then, for any realization ω with density $p(\omega)$ there is a symmetrical realization $\omega' = s\omega$ such

that $p(\omega') = p(\omega)$ and $\omega'(-x) = \omega(x)$ and, by the symmetry of the boundary conditions, $\psi_{\omega'}(-x, -\mathbf{v}) = \psi_\omega(x, \mathbf{v})$. Clearly, $\Omega_k(-x) = s\Omega_k(x)$ and we conclude

$$\psi_k(x, \mathbf{v}) = \int_{\Omega_k(x)} \psi_\omega(x, \mathbf{v}) p(\omega) d\omega = \int_{\Omega_k(-x)} \psi_\omega(-x, -\mathbf{v}) p(\omega) d\omega = \psi_k(-x, -\mathbf{v}).$$

This symmetry is preserved by the LP equations but fails for the MLP model.

4.6 Positiveness

Because the collision operator is positive, the analysis of positiveness may be done considering a punctual source or a boundary flux (a surface source). We consider the following LP or MLP equation with constant cross sections and uniform statistics:

$$(\mu\partial_x + A)\overrightarrow{\psi} = \delta(x - x_0)\overrightarrow{S}, \quad x_L \leq x, x_0 \leq x_R, \tag{16}$$

where $\overrightarrow{\psi} = \{< \psi_k >, k = 1, 2\}$ represents the material fluxes for a bimaterial Markovian mixture, $\overrightarrow{S}(\mu)$ is the source and

$$A = \begin{pmatrix} a_1 & -b_1 \\ -b_2 & a_2 \end{pmatrix}. \tag{17}$$

Here, for the MLP model, $a_k = \Sigma_k + \mu/\lambda_k$ and $b_k = \mu/\lambda_k$, while for the LP model one has to change μ by $|\mu|$ in these expressions.

For simplicity we assume that the cross sections are constant and the statistics uniform so that A is a constant matrix. Then, the solution of (16) is

$$\overrightarrow{\psi}(x, \mu) = \frac{1}{2} sg(x - x_0) e^{-A(x-x_0)/\mu} \frac{\overrightarrow{S}(\mu)}{\mu},$$

where $sg(x)$ is the sign of x.

Because $(x - x_0)/\mu, sg(x - x_0)/\mu > 0$, positiveness rest on the matrix $T = e^{-A(x-x_0)/\mu}$. By using the fact that A can be diagonalized (see Appendix C) we can write:

$$T = M^{-1} \begin{pmatrix} t_+ & \\ & t_- \end{pmatrix} M,$$

where $t_\pm = e^{-\lambda_\pm(x-x_0)/\mu}$, $\lambda_+ > \lambda_-$ are the eigenvalues of A and

$$M = \begin{pmatrix} b_1 & b_1 \\ a_1 - \lambda_+ & \lambda_+ - a_2 \end{pmatrix}.$$

Here M is the matrix, $\overrightarrow{\psi} = M\overrightarrow{\xi}$, that gives the components of a vector on the canonical basis, $\mathbf{e}_k$, in terms of its components $\overrightarrow{\xi} = \{\xi_k, k = 1, 2\}$ on the basis of the eigenvectors of matrix A, $\mathbf{e}_\pm = b_1\mathbf{e}_1 + (a_1 - \lambda_\pm)\mathbf{e}_2$,

After a little bit of algebra we obtain

$$T = \frac{1}{\Delta} \begin{pmatrix} (t_+ + t_-)\lambda_+ - (t_+a_2 + t_-a_1) & (t_- - t_+)b_1 \\ (t_- - t_+)b_2 & (t_+ + t_-)\lambda_+ - (t_+a_1 + t_-a_2) \end{pmatrix},$$

where Δ^2 is the discriminant in (21).

By using the fact that $\lambda_+ > \max(a_1, a_2)$ we see that the diagonal terms of T are positive. Also, $t_- > t_+$ and for the LP model, for which $b_k > 0$, the off-diagonal terms are also positive. On the other hand, for the MLP model the off-diagonal elements of T are positive for $\mu > 0$ and negative for $\mu < 0$. This proves that, with positive sources and boundary fluxes, the LP model will always give positive fluxes, while the MLP model adds negative components to the fluxes, for the sources, boundary fluxes or collisions at positions $x_0 > x$. Thus, the MLP equations are not unconditionally positive. The reason is that, for $\mu < -\frac{\Sigma_1+\Sigma_2}{\lambda_1+\lambda_2}\lambda_1\lambda_2$ the lowest eigenvalue λ_- is negative (see Appendix C).

4.7 Summary of comparisons

The previous comparisons can be summarized as follows:

- The LP model is inherently positive and can be applied to any type of geometry, not necessarily slab, it is exact with no scattering, satisfies the atomic mix limit and has the correct form for the diffusion asymptotic limit for atomic mix, while it does not preserve the diffusion limit for strong coupling. On the other hand, numerical exploration has shown that LP is a robust model with predicts the correct ensemble average fluxes with errors of the order of 5% to 10% (Levermore et al.,1988;Zuchuat et al.,1994).

- The MLP model is exact with scattering for the HSSD problem and related full space problems. Otherwise it is never exact with no scattering for particles with $\mu < 0$ (except for problems obtained from the HSSD problem). This model predicts the atomic mix diffusion limit for both strong and atomic mix couplings and preserves the infinite-medium relaxation modes. The model presents an asymmetry in the treatment of the fluxes in directions $\mu > 0$ and $\mu < 0$ that prevents it to preserve the symmetry of the solution when the boundary conditions and statistics are symmetric. Also, the model is not inherently positive and may produce negative fluxes.

5 NUMERICAL EXAMPLES

In Appendix C we have analyzed the numerical solution of the discrete ordinate formulation of the MLP model in a finite slab with uniform cross sections and statistics. The stability of the solution depends on the nature of the eigenvalues $\lambda_\pm$ of matrix A in Eq. (17). While $\lambda_+ > 0$, for the smallest eigenvalue we find $\lambda_- < 0$ whenever $\tau_{max} \leq 2$ or $\tau_{min} \leq \tau_{max}/(\tau_{max} - 1)$, where $\tau_k = \Sigma_k\lambda_k$ is the mean chord optical length for material k. Moreover, as shown in the appendix, a brutal inversion of the entire operator does not always result in a convergent iterative scheme. Nevertheless, we have chosen to apply a straightforward direct inversion with forward source iterations and a simple diamond differencing, while counting on double precision arithmetics to attenuate the instability effects and force convergence, when possible, by diminishing the width of the spatial mesh. As a consequence of the aforementioned problems some of the calculations we run did not converge.

We have run a number of calculations for the problem suite defined by Pomraning for albedo and transmission calculations with a unit isotropic flux illumination on the left boundary of a finite slab (Zuchuat et al.,1994), as well as related source problems. All the results were done with a S_{16} angular approximation

and converged to 10^{-5} in relative precision. The number of spatial cells was automatically adjusted to satisfy a conservative positive criterion so that the cell width satisfied $\Delta_{cell} \leq |\mu_{min}| / (5\Sigma_{max})$. The stability and convergence of the MLP solutions was verified by running the calculations with 20000 regions to obtain identical results. Reference results were obtained from the averaging of 50000 calculations for randomly generated realizations.

We consider first two albedo-transmission problems from Pomraning's suite for a slab of length L=10. The data for problem **1** are $\Sigma_1 = 10/99$, $\Sigma_2 = 100/11$, $c_1 = 1$, $c_2 = 0$, $\lambda_1 = 99/10$ and $\lambda_2 = 11/10$, $\Sigma_1 = 10/99$, while for problem **2**, $\Sigma_1 = 2/101$, $\Sigma_2 = 200/101$, $c_1 = 0.9$, $c_2 = 0.9$, $\lambda_1 = 101/20$ and $\lambda_2 = 101/20$. We note that problem **2** is a problem with density statistics, the very class of statistics for which MLP is exact for a half-space. Results for these problems are shown in Table 1 and Figs. 1 through 6. Curiously enough, the results show that MLP is better than LP for problem **1** while it is worse than LP for problem **2**.

Finally, in Table 2 and Figs. 7 through 9, we present results for a slab problem (problem **3**) with density sources. The data is the same as for problem 2, except that the entering fluxes are zero and the sources are $S_1 = 0.01$ and $S_2 = 1$.

Although for problem 2 the MLP ensemble and material fluxes are positive, we observed that 40% of the angular fluxes were negative at convergence. This value increased to 52% for problem 3, for which the scalar fluxes become negative. Propagation of negative fluxes in MLP is due to particles emitted in negative directions by the sources (scattering of externals). For problem 2, particles enter the left side of the slab and the main contribution to the scalar fluxes is from particles moving with positive directions, so the scalar fluxes remain positive. However, for problem 3 the particles appear uniformly and isotropically in the slab and therefore particles traveling left can overcome those traveling right and the result are negative scalar fluxes on the left of the slab, as shown in Figs. 7 and 8.

Table 1: Albedos β and transmissions t for problems **1** and **2**.

problem		reference	LP	MLP
1	β	4.34546×10^{-1}	2.90962×10^{-1}	3.11812×10^{-1}
	t	1.85351×10^{-1}	1.94468×10^{-1}	1.94569×10^{-1}
2	β	4.46270×10^{-1}	3.27217×10^{-1}	1.05145×10^{-1}
	t	1.04333×10^{-1}	1.19473×10^{-1}	1.33489×10^{-1}

Table 2: Problem **3**. Left and right exiting currents.

J^{out}	reference	LP	MLP
Left	5.69116×10^{-1}	7.00687×10^{-1}	-3.11368
Right	5.69116×10^{-1}	7.00687×10^{-1}	9.64264×10^{-1}

6 CONCLUSIONS

Our numerical comparisons between the LP model and the MLP with natural boundary conditions show that MLP behaves well when the bulk of the particles move in positive directions, although we observed

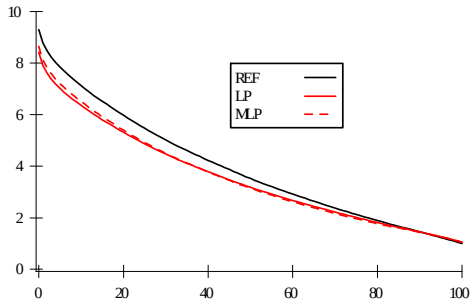

Figure 1. Problem **1**. Ensemble average fluxes.

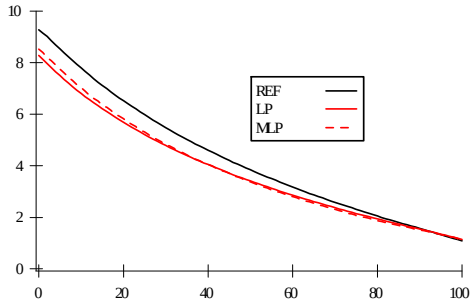

Figure 2. Problem **1**. Material fluxes for material 1 (ψ_1) .

a fair amount of negative angular fluxes. However, in the presence of uniform and isotropic sources, the lack of positiveness and symmetry of MLP shows deleterious effects in the form of negative fluxes. Akcasu (Akcasu,2007a,2007b) proposes to use different boundary conditions to compute source problems, but then the MLP solution does not exactly satisfy the natural boundary conditions of the problem and, although the ensemble average entering currents is zero, the material averages of the entering currents on the right surface are non zero. Furthermore, the material fluxes can become negative. It is clear that much work needs to be done in order to define approximated boundary conditions that give satisfactory results when using MLP in finite slabs.

Our opinion is that at present time one does not know how to obtain an improved model from the LP and MLP equations. Such a model should retain the robust properties of LP (symmetry, positiveness, exact non scattering limit) while adding a better treatment for collisions and preserving the MLP equations for the HSSD problem.

Another possibility could be to derive a better closure of the exact equations (Adams et al.,1989; Sanchez,1989) by using MLP to obtain an improved approximation for the interface fluxes. By comparing the exact equations with MLP for the HSSD problem, one realizes that, in this particular situation,

$$\begin{aligned} < \psi_{j\to i}(x,\mu) > &= < \psi_j(x,\mu) >, \quad \mu > 0, \\ < \psi_{j\to i}(x,\mu) > &= < \psi_i(x,\mu) >, \quad \mu < 0, \end{aligned} \tag{18}$$

where $< \psi_{j\to i}(x,\mu) >$ is the ensemble average of the flux over all realizations that transit at x in direction

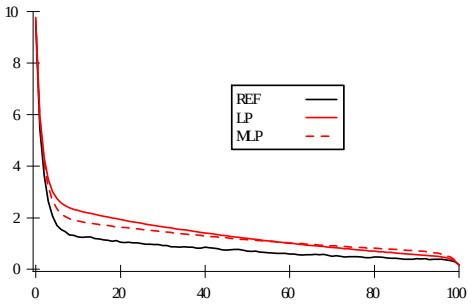

Figure 3. Problem **1**. Material fluxes for material 2 (ψ_2).

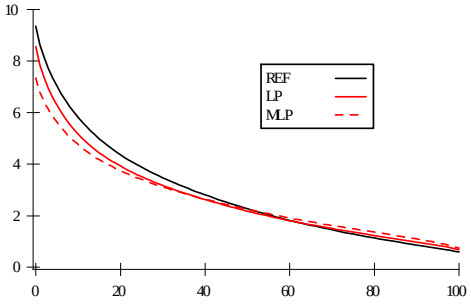

Figure 4. Problem **2**. Ensemble average fluxes.

μ from material j into material i, and $< \psi_i(x,\mu) >$ are the ensemble averaged material fluxes.

This is an interesting find in itself, but this property is not satisfied by finite slabs of for half-slabs with other type of statistics different from density statistics. Formula (18) holds only for density statistics in a half-space, and it is not clear how this property can be used to define a closure for the interface fluxes $< \psi_{j\to i}(x,\mu) >$ for more realistic problems.

A simple approach may consists of deriving a heuristic model based on an interpolation formula of the following form:

$$\begin{aligned} < \psi_{j\to i}(x,\mu) > &= < \psi_j(x,\mu) >, & \mu > 0, \\ < \psi_{j\to i}(x,\mu) > &= \alpha_{ji} < \psi_i(x,\mu) > + (1-\alpha_{ji}) < \psi_j(x,\mu) >, & \mu < 0, \end{aligned}$$

where α_{ji} is a function of the material properties, mean chord lengths and width L of the slab such that $0 \le \alpha_{ji} \le 1$, $\alpha_{ji} = 0$ when $c_i = c_j = 0$ and $\alpha_{ji} = 1$ in the conditions of the HSSD problem . The simpliest function of this type is $\alpha_{ji} = (c_i + c_j)/(ae^{-L} + c_i + c_j)$, where $a > 0$ is a parameter. Such an interpolation will give the good limit for pure ansorption and the MLP limit with collisions.

ACKNOWLEDGEMENTS

Many thanks are due to Ed Larsen and Ziya Akcasu for comments and discussions, as well as for providing unpublished material. Although there has been much controversy and our opinions are sometimes drastically

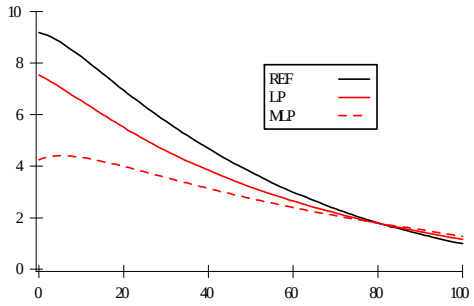

Figure 5. Problem **2**. Material fluxes for material 1 (ψ_1).

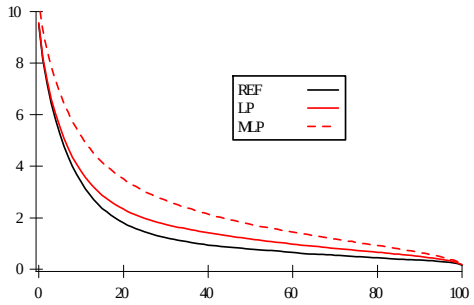

Figure 6. Problem **2**. Material fluxes for material 2 (ψ_2).

different, the email exchanges helped me to understand better MLP. Clearly, the opinions advanced in this paper are the sole responsibility of the author.

APPENDIX A: DERIVATION OF THE MASTER EQUATION FOR THE $P_k(\tau; x)$

Consider the value of $P_k(\tau; x + \Delta x)$. Because (τ, ω) is a Markovian process, for Δx small, we can write $P_k(\tau; x + \Delta x)$ in terms of P_k and $P_{k'}$ at x. The realizations that contribute to $P_k(\tau; x + \Delta x)$ are those that have material k at $x + \Delta x$ with $\tau(x, \omega) \in (\tau, \tau + d\tau)$. These realizations either have material k at x and keep this material in $(x, x + \Delta x)$ with probability $1 - \Delta x/\lambda_k$, or have material k' at x and change to material k in $(x, x + \Delta x)$ with probability $\Delta x/\lambda_{k'}$. Thus

$$P_k(\tau; x + \Delta x) = P_k(\tau - N_k \Delta x; x)(1 - \Delta x/\lambda_k) + P_{k'}(\tau - N_{k'} \Delta x; x)\Delta x/\lambda_{k'} + O((\Delta x)^2).$$

Next, we subtract $P_k(\tau; x)$ from both sides of this expression, divide by Δx and take the limit for $\Delta x \to 0$. The result is

$$\begin{aligned}(\partial_x P_k)(\tau; x) &= \lim_{\Delta x \to 0_+} \frac{1}{\Delta x}[P_k(\tau; x + \Delta x) - P_k(\tau; x)] \\ &= -P_k(\tau; x)/\lambda_k(x) + P_{k'}(\tau; x)/\lambda_{k'}(x) - \lim_{\Delta x \to 0_+} \frac{1}{\Delta x}[P_k(\tau; x) - P_k(\tau - N_k \Delta x; x)].\end{aligned}$$

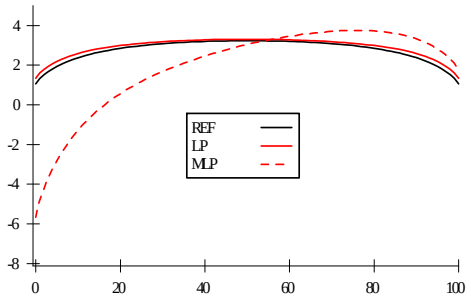

Figure 7. Problem **3**. Ensemble average fluxes.

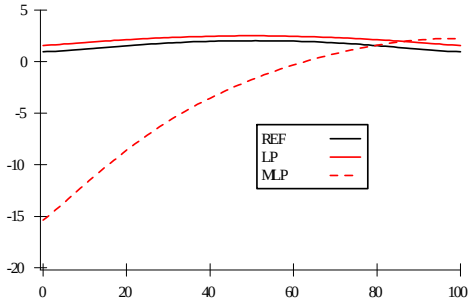

Figure 8. Problem **3**. Material fluxes for material 1 (ψ_1).

Finally, by recognizing that the limit on the right-hand-side can be written as $\lim_{\Delta\tau\to 0_+} \frac{1}{\Delta\tau} N_k[P_k(\tau;x) - P_k(\tau-\Delta\tau;x)]$ we obtain the final expression:

$$(\partial_x P_k)(\tau;x) = -P_k(\tau;x)/\lambda_k(x) + P_{k'}(\tau;x)/\lambda_{k'}(x) - \partial_\tau(N_k P_k)(\tau;x).$$

APPENDIX B: CONSTRUCTION OF THE PROPAGATOR

The solution of the finite slab problem with incoming boundary condition and no sources can be written as

$$\psi(x,\mathbf{v}) = \int dE' \int_0^1 \mu' d\mu' [g(x_L,\mathbf{v}'\to x,\mathbf{v})\psi^L_{in}(\mathbf{v}') + g(x_R,-\mathbf{v}'\to x,\mathbf{v})\psi^R_{in}(-\mathbf{v}')], \qquad (19)$$

where $g(x_L,\mathbf{v}'\to x,\mathbf{v})$ and $g(x_R,\mathbf{v}'\to x,\mathbf{v})$ are the Green's functions for particles entering the left (L) or the right (R) surfaces of the slab and zero incoming fluxes on the opposite surface.

We write this equation as

$$\psi(x,\mathbf{v}) = (G^L\psi^L_{in})(x,\mathbf{v}) + (G^R\psi^R_{in})(x,\mathbf{v})$$

where G^L and G^R are the integral operators in (19). In order to derive the propagator formulation in (12) one needs to write $\psi^R_{in}(\mathbf{v})$ in terms of the flux exiting the left boundary. If the operator $G^{LR} = G^R(x_L,\mathbf{v})$ has an inverse over the domain $\mu < 0$ we obtain

$$\psi(x,\mathbf{v}) = ([G^L - G^R(G^{LR})^{-1}G^{LL}]\psi^L_{in})(x,\mathbf{v}) + (G^R(G^{LR})^{-1}\psi^L_-)(x,\mathbf{v}),$$

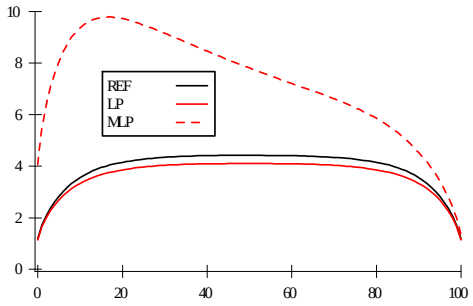

Figure 9. Problem **3**. Material fluxes for material 2 (ψ_2).

where $G^{LL} = G^L(x_L, \mathbf{v})$ and $\psi_-^L(\mathbf{v})$ denotes the flux exiting the left surface.

Note that the propagator formulation depends on the existence of the inverse of operator G^{LR}. As an aside comment we note that this is equivalent to the uniqueness of the inverse problem $\psi_-^L(\mathbf{v}) \rightarrow \psi_{in}^R(\mathbf{v})$ for a finite slab. Moreover, as our construction shows, calculation of the propagator is equivalent to the computation of the Green's functions and therefore of the complete solution of the problem.

APPENDIX C: NUMERICAL SOLUTION FOR THE MLP MODEL

We investigate the solution of the MLP equations by source iterations based on a discrete ordinates approximation. By introducing the two-dimensional vectors $\overrightarrow{\psi} = \{< \psi_k >, k = 1, 2\}$ and $\overrightarrow{q} = \{H_k < \psi_k > + S_k, k = 1, 2\}$ we write the power iteration process as

$$(\mu\partial_x + A)\overrightarrow{\psi}_n = \overrightarrow{q}_{n-1}, \tag{20}$$

where n is the iteration index and, for homogeneous statistics and cross sections and A is the matrix in (17).

Stability

Next, to investigate the stability of the iterations, we look for the eigenvalues of matrix A. These are given by $\lambda_\pm = (b \pm \Delta)/2$ where

$$\begin{aligned} b &= \Sigma_1 + \Sigma_2 + \mu(1/\lambda_1 + 1/\lambda_2), \\ c &= \Sigma_1\Sigma_2 + \mu(\Sigma_2/\lambda_1 + \Sigma_1/\lambda_2) \end{aligned}$$

and

$$\Delta^2 = b^2 - 4c = [\Sigma_1 - \Sigma_2 - \mu(1/\lambda_1 - 1/\lambda_2)]^2 + 4\mu^2/(\lambda_1\lambda_2) \geq 0. \tag{21}$$

Thus, the two eigenvalues are real and different and A is diagonalizable.

We consider first the case of the LP model where one has to replace μ by $|\mu|$ in the expressions for b, c and Δ. For this case one finds that the two eigenvalues are positive and, therefore, the stable power iteration strategy for (20) is to solve for increasing x values for $\mu > 0$ and for decreasing x values for $\mu < 0$.

However, for the MLP operator we have two different cases that depend on the signs of c and b. Let us define the mean optical chord length

$$\tau_k = \Sigma_k \lambda_k.$$

Then, coefficients c and b are negative in the following ranges

$$\begin{array}{ll} c<0, & \mu < \mu_c = -\frac{\tau_1\tau_2}{\tau_1+\tau_2}, \\ b<0, & \mu < \mu_b = -(p_2\tau_1 + p_1\tau_2), \end{array}$$

where $\mu_b < \mu_c < 0$. We have, therefore, two different domains:

a) For $\mu > \mu_c$ the two eigenvalues are positive and the stable strategy is to do a forward sweep,

b) For $\mu < \mu_c$ one eigenvalue is positive and the other negative. In this case, Eq. (20) has to be diagonalized and the sweep done independently for each eigenvalue. The stable strategy for the positive eigenvalue is the forward sweep, while the stable strategy for the negative eigenvalue is the backward sweep. At $\mu = \mu_c$ the smallest eigenvalue is 0, while at $\mu = \mu_b$ the two eigenvalues are equal and of opposite sign.

For a negative eigenvalue, stability requires sweeping along the backward trajectory starting with an exiting angular flux. Because this flux is not known one will have to set up a shooting technique that, via iterations, will produce the good incoming flux at the opposite boundary. By using linearity this requires only two iterations. In the first one runs the backward sweep setting the initial escaping flux ψ_{out} to 1, and computes separately the contributions from the internal sources, $\psi_{in}(q)$, and from the boundary flux, $\psi_{in}(\psi_{out}=1)$, to the flux ψ_{in} entering the opposite boundary. The correct exiting flux value is given by $\psi_{out} = (\psi_{in} - \psi_{in}(q))/\psi_{in}(\psi_{out} = 1)$. It suffices then to redo the backward sweep using the correct value of ψ_{out}. Because this procedure for stable iterations is cumbersome, in a first time we shall use the standard iteration procedure that sweeps always along the forward direction, starting with the known boundary fluxes. For a negative eigenvalue λ this gives for the transmitted flux:

$$\psi(x,\mu) = e^{-\lambda x/\mu}\psi^L_{in}(\mu),\ \mu > 0$$

where the positive exponential magnifies any errors due to finite precision arithmetic operations. Note, however, that the relative precision on the solution,

$$\delta\psi/\psi = \delta\psi^L_{in}/(\psi^L_{in} + \delta\psi^L_{in}),$$

remains bounded. Therefore, for finite slabs, for which the magnifying factor is bounded, it is possible, by increasing the precision of the calculation if necessary, to obtain correct results. If an increase of the precision (number of digits used in the calculation) does not stabilize the problem, then one can resort to the more complicated shooting scheme first discussed.

Convergence of power iterations

Consider the discrete-ordinates diamond-differencing form of Eq. (20) with a mesh of constant width Δ:

$$\begin{array}{c} (\frac{2|\mu|}{\Delta} + A)\,\overrightarrow{\psi}_n = \frac{2|\mu|}{\Delta}\overrightarrow{\psi}_{n,-} + \overrightarrow{q}_{n-1}, \\ \overrightarrow{\psi}_{n,+} = 2\overrightarrow{\psi}_n - \overrightarrow{\psi}_{n,-}, \end{array} \tag{22}$$

where $\overrightarrow{\psi}_n$ and $\overrightarrow{q}_{n-1}$ are cell-averaged values and $\overrightarrow{\psi}_{n,\pm}$ are the cell exiting $(+)$ or entering $(-)$ fluxes. In our implementation of source iterations we have adopted the previous scheme. Contrarily to the LP model, for $\mu < 0$ the MLP model weakens the diagonal terms of matrix $\frac{2|\mu|}{\Delta} + A$ and this may result in non convergence of the iterations. Several techniques can be used to resolve this problem: Wrapping around a Krylov solver (Fichtl et al.,2006), adopting a convergent splitting $A = A_+ - A_-$ and iterating also on term $A_- \overrightarrow{\psi}_{n-1}$ and, more simply but less efficient, decrease the cell width Δ. To use a Krylov solver (GMRES) one would write the iterations as $\overrightarrow{\Phi} = HL^{-1}(\overrightarrow{\Phi} + \overrightarrow{S})$, where $L = 2|\mu|/\Delta + A$, H is the scattering operator, $\overrightarrow{S}$ the source and $\overrightarrow{\Phi} = H\overrightarrow{\psi}$ are the angular flux moments. However, in our tests we have opted for the expedient solution of diminishing the cell width.

Fourier analysis

This is another way to look at convergence. For an infinite slab of identical, homogeneous cells we introduce the Fourier anszats $\overrightarrow{\psi}_n(x,\mu) \sim \overrightarrow{\psi}_n(\omega,\mu) \times \exp(i\omega\Delta n)$ and $\overrightarrow{\psi}_{n,+}(x,\mu) \sim \overrightarrow{\psi}_{n,bd}(\omega,\mu)\exp(i\omega\Delta n)$ for the cell averaged flux and the exiting fluxes for cell n to obtain:

$$\overrightarrow{\Phi}_n(z) = M(z)c\overrightarrow{\Phi}_{n-1}(z),$$

where we have assumed isotropic scattering $\overrightarrow{q}(x,\mu) = c\Sigma\overrightarrow{\Phi}(x)$ with $c = diag\{c_1, c_2\}$, $\Sigma = diag\{\Sigma_1, \Sigma_2\}$ and $\overrightarrow{\Phi}(x) = (1/2)\int_{-1}^{1}\overrightarrow{\psi}(x,\mu)d\mu$, $z = (\omega\Delta)/2$ and $M(z) = \frac{1}{2}\int_{-1}^{1} M(z,\mu)d\mu$. In the last expression the matrix $M(z,\mu)$ is

$$M(z,\mu) = \frac{1}{D(z,\mu)}\begin{pmatrix} 1+\mu(a_2+ib_2) & \mu a_1 \\ \mu a_2 & 1+\mu(a_1+ib_1) \end{pmatrix}$$

with $a_k = 1/\tau_k$, $b_k = f(z)/(\Sigma_k\Delta)$, $f(z) = 2\tan z$ and

$$D(z,\mu) = 1 + \mu(a_1 + ib_1 + a_2 + ib_2) + \mu^2[i(a_1b_2 + a_2b_1) - b_1b_2].$$

The function $f(z)$ is periodic with period π and has the symmetry property $f(z) = -f(\pi - z)$. The function behaves as z for $z \to 0$ and increases monotonously from 0 at $z = 0$ to ∞ at $z = \pi/2$ where it has a vertical asymptote. Because of the periodicity the spectral radius of the iterator is given by $\rho_M = \max_{0\le z\le\pi}(|\lambda_+(z)|, |\lambda_-(z)|)$. In the last expression $\lambda_\pm(z) = (b \pm \Lambda)/2$ are the eigenvalues of $M(z)c$ with

$$b = (c_1 + c_2)I_0 + [c_1(a_2 + ib_2) + c_2(a_1 + ib_1)]I_1,$$
$$\Lambda^2 = [(c_1 - c_2)I_0 + [c_1(a_2 + ib_2) - c_2(a_1 + ib_1)]I_1]^2 + 4c_1c_2a_1a_2I_1^2,$$

where $I_p(z) = (1/2)\int_{-1}^{1}\mu^p d\mu/D(z,\mu)$.

From here on the analysis has to be done by numerical evaluation and is out of the scope of this work. An analytical result can be obtained for the flat modes ($\omega = 0$) when $c_1 = c_2 = c$: For $\Delta > 0$ let us look at the eigenvalues $\lambda_\pm(z)$ at $z = 0$. One finds $\lambda_+(0) = c$ and $\lambda_-(0) = cI_0(0) = (c/2)\ln[(1+x)/(1-x)]$, where $x = a_1 + a_2$. Thus, with equal c_k values, power iterations will converge the flat modes in an infinite slab if $1/\tau_1 + 1/\tau_2 < (e^2-1)/(e^2+1) \simeq 0.7616$. Another interesting case, regarding Pomraning's test problems, is for $c_1 = 0$. Here, for $\Delta > 0$ and $z = 0$ we find $\lambda_+(0) = c_2[\tau_1 I_0(0) + \tau_2]/(\tau_1 + \tau_2)$ and $\lambda_-(0) = 0$.

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