STATE OF ART OF PARTICLE TRANSPORT THEORY IN STOCHASTIC MEDIA

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Abstract. In this work we report the state of art of particle transport theory in stochastic media, discussing in detail the derivation of the atomic mix and the Levermore-Pomraning models. We consider time independent stochastic transport in a randomly mixed binary medium. A Monte Carlo procedure is used to generate a physical realization of the statistics, and for this realization we numerically solve the transport equation, using the LTS_N formulation. The ensemble-averaged solution, as well as the standard deviation, is obtained by averaging a large number of such calculations. Then, we compare this solution with those obtained for the atomic mix and the Levermore-Pomraning models.

Keywords: Transport Theory, Stochastic Media, Atomic Mix, Levermore-Pomraning

1. INTRODUCTION

The description of linear particle transport and radiative transfer in a stochastic medium consisting of two randomly immiscible materials has been an important recent problem in transport theory. If we write the transport equation as

$$\begin{aligned}\frac{1}{v}\frac{\partial\psi}{\partial t}(r,E,\Omega,t)+\Omega\cdot\nabla\psi(r,E,\Omega,t)+\Sigma_t(r,E,t)\psi(r,E,\Omega,t)=\\ =\int_0^\infty\int_{4\pi}\Sigma_s(r,E'\to E,\Omega'\cdot\Omega,t)\psi(r,E',\Omega',t)d\Omega' dE'+Q(r,E,\Omega,t),\end{aligned} \tag{1}$$

the goal has been to develop a formalism to describe the ensemble-averaged solution to this equation, when Σ_t, Σ_s and Q are binary discrete random variables. Here, $\psi(r,E,\Omega,t)$ is the angular flux, with r, Ω, and t representing the spatial, angular, and time coordinates, and E representing the particle's energy; v is the particle speed; $\Sigma_t(r,E,t)$ is the total cross section; $\Sigma_s(r,E'\to E,\Omega'\cdot\Omega,t)$ is the scattering kernel (such that $\Sigma_s(r,E,t)$ is the scattering cross section); and $Q(r,E,\Omega,t)$ represents an internal source of particles. Further, assuming that the system of interest is nonreentrant (convex) and characterized by a volume V, and that the range of interest in the time variable is $0\le t<\infty$, Eq. (1) is subject to the boundary and initial conditions

$$\psi(r_s,E,\Omega,t)=\Gamma(r_s,E,\Omega,t)\quad n\cdot\Omega<0, \tag{2}$$

$$\psi(r,E,\Omega,0)=\alpha(r,E,\Omega), \tag{3}$$

where Γ and α are specified functions, r_s is a point on the surface, and n is a unit outward normal vector at this point.

Historically, this problem has been solved through a widely-used approximate homogenization technique known as *Atomic Mix*, which is valid when the system's spatial heterogeneities occur on a length scale which is small compared to a typical mean free path. The term atomic mix applies to mixtures of two or more materials in which the "chunks" of the materials are so small that we can assume mixing at the atomic level. Its derivation can be intuitively done, since this assumption leads us to think of a homogeneous material with physical parameters given by the average of each component material properties.

Bearing in mind the limitation of this assumption, a formulation of a particle transport formalism in binary random media arised in the mid-1980's, providing the foundations for the so-called Levermore-Pomraning method. The first derivations of the Levermore-Pomraning method (Levermore et al., 1986; Pomraning, 1986) considered time independent transport in a purely absorbing medium. In this case, an exact solution was obtained for the ensemble-averaged angular flux. However, this derivation becomes algebraically too cumbersome to lead to useful results when the scattering interaction is involved (Pomraning, 1991). In fact, in scattering problems, the task of reducing this exact expression to an useable one is exceedingly complex.

Later, it was shown (Vanderhaegen, 1986) that the use of Chapman-Kolmogorov equations (Parzan, 1962; Pomraning, 1991) provides a master equation for the joint probability density (Frisch, 1968; Morrison, 1972; Van Kampen, 1981). This treatment was extended by a master equation approach to analyze the general transport equation, including time dependence and scattering.

In this work, we discuss still another derivation of this model, using the idea of the stochastic balance, introduced by Adams et al. (1989). Here, however, the details of the derivation are

done in a different way, in such manner that the reader may find it more illuminating in terms of the physics of the problem.

We outline this paper as follows: in section 2, we briefly present the physical problem, and derive the atomic mix equation for the case of nonscattering transport, which can be readily extended to the general case. At the end of the section we remark that, despite its simplicity, the atomic mix model shows itself very innacurate when its basic assumption is not satisfied. In section 3, we derive the Levermore-Pomraning equations using the stochastic balance idea, reporting in detail all the derivation steps as well as underlying physical assumptions. In section 4, we consider time independent stochastic transport (including scattering) in a layered planar geometry, under the assumption of homogeneous Markov mixing statistics for the two components of the random medium. We generate a physical realization of the statistics using a Monte Carlo procedure, and numerically solve the corresponding transport equation. We repeat this process a large number of times and average the results. The physical problem we consider is the transmission-reflection problem for a finite system without internal sources. We report the ensemble-averaged probabilities of reflection and transmission, as well as their respective standard deviations, for different choices of Σ_t, Σ_s and slab thickness. Then, we compare the predictions of the atomic mix and Levermore-Pomraning models with these results.

2. THE ATOMIC MIX MODEL

Let us consider neutron transport in a heterogeneous volume V such that the boundary ∂V of V is specified, but the interior structure of V is unknown. Specifically, we restrict our attention to the case in which V consists of two random immiscible materials denoted by an index i, with $i = 1, 2$. We can actually imagine V as a heterogeneous volume consisting of randomly distributed chunks of random sizes and shapes of material 1 imbedded in material 2. If we consider a particle traversing the mixture along a random path, it will pass through alternating segments of these two materials, as we can see in Fig. 1.

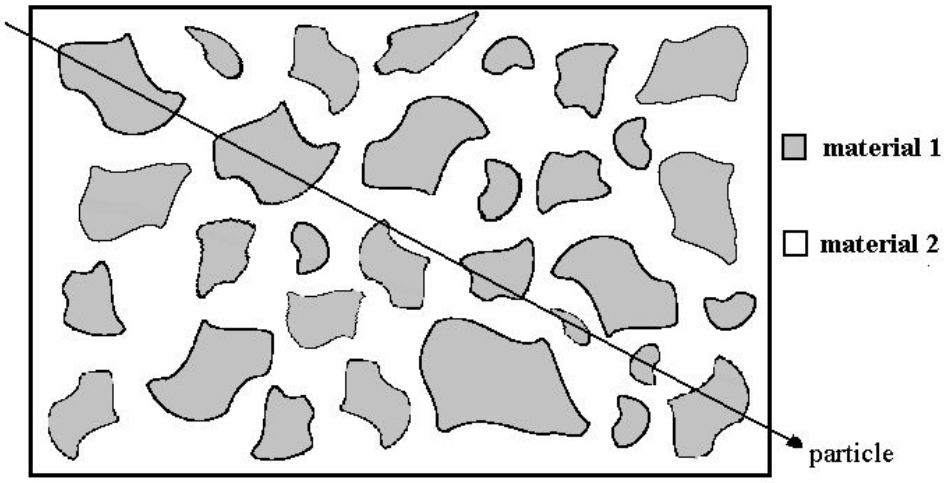

Figure 1: Particle traversing the mixture along a random path

The quantities Σ_t, Σ_s and Q are considered as discrete random variables. That is, in the ith material, these elements are denoted by $\Sigma_{ti}(r, E, t)$, $\Sigma_{si}(r, E' \to E, \Omega' \cdot \Omega, t)$, and $Q_i(r, E, \Omega, t)$. Thus, the stochasticity of the problem is due to the fact that we only have a probabilistic idea about which material ocuppies the space point r at a time t. Since we consider Σ_t, Σ_s and Q as random variables, we must also consider the angular flux ψ as a random variable. Therefore, we want to find an expression for $\langle \psi \rangle$, the ensemble-averaged angular flux, i.e., the expected

value of ψ.

For convenience, let us consider the case of transport in a nonscattering medium. Thinking about $\Omega \cdot \nabla$ in Eq. (1) as a directional derivative, and using $\Sigma_t = \Sigma_s + \Sigma_a$, where Σ_a is the absorption cross section, we can rewrite this equation as

$$\frac{1}{v}\frac{\partial \psi(s,t)}{\partial t} + \frac{\partial \psi(s,t)}{\partial s} + \Sigma_a(s,t)\psi(s,t) = Q(s,t), \tag{4}$$

where s denotes the spatial variable in the direction Ω. One must notice that Eq. (4) describes particle transport at each energy E and direction Ω, which are omitted since they are only parameters. We also consider the boundary condition

$$\psi(0,t) = \Gamma(0,t), \tag{5}$$

and the initial condition

$$\psi(s,0) = \alpha(s). \tag{6}$$

We denote $\langle W \rangle$ as the ensemble average of any random variable W, and define $\tilde{W}$ as the deviation of W from $\langle W \rangle$. Then $\langle \tilde{W} \rangle = 0$, and $W = \langle W \rangle + \tilde{W}$. Using this notation, we ensemble-average equations (4) through (6) to obtain

$$\frac{1}{v}\frac{\partial \langle \psi \rangle}{\partial t} + \frac{\partial \langle \psi \rangle}{\partial s} + \langle \Sigma_a \rangle \langle \psi \rangle + \langle \tilde{\Sigma}_a \tilde{\psi} \rangle = \langle Q \rangle, \tag{7}$$

$$\langle \psi(0,t) \rangle = \langle \Gamma(0,t) \rangle = \Gamma(0,t), \tag{8}$$

$$\langle \psi(s,0) \rangle = \langle \alpha(s) \rangle = \alpha(s). \tag{9}$$

The values of $\langle \Sigma_a \rangle$ and $\langle Q \rangle$ in this equation are defined in terms of the properties of materials 1 and 2. Defining $p_i(s,t)$ as the probability of presence of the material i at position s at time t, such that

$$p_1(s,t) + p_2(s,t) = 1, \tag{10}$$

we can write

$$\langle \Sigma_a(s,t) \rangle = p_1(s,t)\Sigma_{a1}(s,t) + p_2(s,t)\Sigma_{a2}(s,t), \tag{11}$$

$$\langle Q(s,t) \rangle = p_1(s,t)Q_1(s,t) + p_2(s,t)Q_2(s,t), \tag{12}$$

Now, let us define the characteristic chord length for the chunks of the material i as Λ_i. Assuming that

$$\Sigma_{ti}\Lambda_i \ll 1, \quad i = 1,2, \tag{13}$$

then a particle, between collisions, is likely to travel a distance that spans many different chunks of materials 1 and 2. Since $\Sigma_{ti} = \lambda_i^{-1}$ (where λ_i is the mean free path of material i), Eq. (13) means that Λ_i is very small when compared with λ_i. On physical grounds, this assumption appropriately describes vanishingly small chunks in the mixture, which can be understood as if the two components of the system were mixed at the atomic level. In the present case we have $\Sigma_{ti} = \Sigma_{ai}$, and therefore it is clear that the cross correlation term $\langle \tilde{\Sigma}_a \tilde{\psi} \rangle$ in Eq. (7) can be neglected when Eq. (13) is valid. Thus, Eq. (7) becomes

$$\frac{1}{v}\frac{\partial \langle \psi \rangle}{\partial t} + \frac{\partial \langle \psi \rangle}{\partial s} + \langle \Sigma_a \rangle \langle \psi \rangle = \langle Q \rangle, \tag{14}$$

which is closed for the ensemble-averaged angular flux $\langle\psi\rangle$. This equation represents the atomic mix description of Eq. (4) (nonscattering media).

Applying the same arguments above on equations (1) through (3), the atomic mix description of stochastic transport, including scattering, is given by

$$\begin{aligned}\frac{1}{v}\frac{\partial\langle\psi(r,E,\Omega,t)\rangle}{\partial t}+\Omega\cdot\nabla\langle\psi(r,E,\Omega,t)\rangle+\langle\Sigma_t(r,E,t)\rangle\langle\psi(r,E,\Omega,t)\rangle=\\ =\int_0^\infty\int_{4\pi}\langle\Sigma_s(r,E'\to E,\Omega'\cdot\Omega,t)\rangle\langle\psi(r,E',\Omega',t)\rangle d\Omega' dE'+\langle Q(r,E,\Omega,t)\rangle,\end{aligned} \tag{15}$$

with

$$\langle\psi(r_s,E,\Omega,t)\rangle=\Gamma(r_s,E,\Omega,t),\qquad n\cdot\Omega<0, \tag{16}$$

$$\langle\psi(r,E,\Omega,0)\rangle=\alpha(r,E,\Omega). \tag{17}$$

Here, for any random variable W we have

$$\langle W\rangle=p_1(r,t)W_1+p_2(r,t)W_2, \tag{18}$$

and the neglected cross correlation terms are $\langle\tilde{\Sigma}_t\tilde{\psi}\rangle$ and $\langle\tilde{\Sigma}_s\tilde{\psi}\rangle$.

REMARK:

Atomic mix is a very appealing model because of its simplicity. Since the cross correlation terms are neglected, this model leads to a description that essentialy does not deal with stochastic effects. Assuming that the statistics of mixing is known, the problem of solving Eq. (15) is not different of the one we face to solve Eq. (1). However, when Eq. (13) is not satisfied, the atomic mix description is generally inaccurate. Although there exist specified classes of problems in which atomic mix is shown to be accurate even when the chunk sizes are not optically small (Larsen, 2003), in general it fails quite badly in these situations. As an example, consider time independent transport in a nonscattering medium without internal sources, given by

$$\frac{\partial\psi(s)}{\partial s}+\Sigma_a(s)\psi(s)=0, \tag{19}$$

with the boundary condition

$$\psi(0)=\Gamma_0, \tag{20}$$

where ($0\le s<\infty$). Following Pomraning (1991), let material 1 be composed of optically thin packets such that $\Sigma_{a1}\Lambda_1\ll 1$. Then, define material 2 as very sparse optically thick chunks imbedded on material 1, in such way that $\Sigma_{a2}\Lambda_2\gg 1$ and $p_2(s)\ll 1$. Here, Λ_i is the characteristic chord length of material i and p_2 is the probability of finding material 2 at position s. The physical description is that of a near vacuum where sparse absorbing packets of (essentialy) infinite thickness can be found. Particles travelling through this mixture tend to pass through it without undergoing an interaction, at least on the average, as can be seen from Fig. 2. On the other hand, if we write the atomic mix description of equations (19) and (20) neglecting the cross correlation term $\langle\tilde{\Sigma}_a\tilde{\psi}\rangle$:

$$\frac{\partial\langle\psi\rangle}{\partial s}+\langle\Sigma_a\rangle\langle\psi\rangle=0, \tag{21}$$

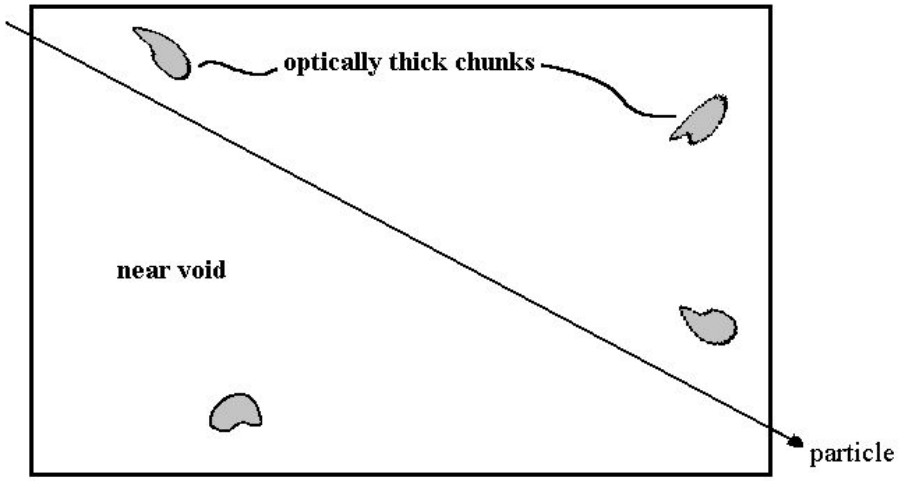

Figure 2: Particle travelling through a near void with sparse chunks

$$\left\langle \psi(0) \right\rangle = \left\langle \Gamma_0 \right\rangle = \Gamma_0, \tag{22}$$

we will conclude that $\left\langle \psi \right\rangle$ will be exponentially attenuated, with a scale length $1/\left\langle \Sigma_a \right\rangle$, and it is clear that $\left\langle \Sigma_a \right\rangle$ is very large, since Σ_{a2} is very large. Therefore, this modelling will lead to essentialy no transmission through the system. In general, the cross correlation term neglecting will always underestimate particle transmission.

3. THE LEVERMORE-POMRANING METHOD

We will now present a derivation of the Levermore-Pomraning equations, restricting our considerations to time independent statistics (i.e., the configuration of materials 1 and 2 in any given physical realization of the mixing statistics is static). Further, the statistics is taken to be homogeneous, by which we mean that all points in the system have the same statistical properties. In this case, the probability of finding material i at point r is given by

$$p_i(r) = \frac{\Lambda_i}{\Lambda_1 + \Lambda_2}, \tag{23}$$

where, again, Λ_i is the characteristic chord length for the chunks of material i.

For notation simplicity, let us consider the transport equation with an isotropic internal source, and let us assume that the scattering process is both coherent and isotropic. Thus, we have

$$\frac{1}{v}\frac{\partial \psi(r,\Omega,t)}{\partial t} + \Omega \cdot \nabla \psi(r,\Omega,t) + \Sigma_t \psi(r,\Omega,t) = \frac{\Sigma_s}{4\pi}\int_{4\pi} \psi(r,\Omega',t)d\Omega' + \frac{Q(r,t)}{4\pi}, \tag{24}$$

and we define boundary and initial conditions

$$\psi(r_s,\Omega,t) = \Gamma(r_s,\Omega,t),\ n\cdot\Omega < 0 \tag{25}$$

$$\psi(r,\Omega,0) = \alpha(r,\Omega), \tag{26}$$

where r_s is a point on the surface of the system and n is a unit outward normal vector at r_s.

Now, we introduce the characteristic functions

$$\chi_i(r) = \begin{cases} 1, & \text{if } r \text{ is in material } i \\ 0, & \text{if } r \text{ is in material } j \neq i \end{cases}. \tag{27}$$

The basic issue is that we do not know the functions $\chi_1(r)$ and $\chi_2(r)$, but we know that they satisfy

$$\chi_1(r) + \chi_2(r) = 1. \tag{28}$$

Multiplying Eq. (24) by $\chi_i(r)$, and using:

$$\chi_i\big(\Omega \cdot \nabla\psi\big) = \Omega \cdot \nabla(\chi_i\psi) - \psi(\Omega \cdot \nabla\chi_i), \tag{29}$$

$$\chi_i\Sigma_t = \Sigma_{ti}\chi_i, \tag{30}$$

$$\chi_i\Sigma_s = \Sigma_{si}\chi_i, \tag{31}$$

$$\chi_i Q = Q_i\chi_i, \tag{32}$$

we find, for $i = 1, 2$,

$$\frac{1}{v}\frac{\partial(\chi_i\psi)}{\partial t} + \Omega\cdot\nabla(\chi_i\psi) + \Sigma_{ti}(\chi_i\psi) = \frac{\Sigma_{si}}{4\pi}\int_{4\pi}\chi_i\psi(r,\Omega',t)d\Omega' + \frac{Q_i\chi_i}{4\pi} + \psi(\Omega\cdot\nabla\chi_i). \tag{33}$$

The next step is to ensemble average this result over all statistical realizations. We obviously have the ensemble-averaged characteristic function given by

$$\big\langle\chi_i(r)\big\rangle = p_i(r), \tag{34}$$

and therefore we define

$$\psi_i(r,\Omega,t) = \frac{\big\langle\chi_i(r)\psi(r,\Omega,t)\big\rangle}{\big\langle\chi_i(r)\big\rangle}, \tag{35}$$

where ψ_i is the ensemble average of $\psi(r,\Omega,t)$ over all physical realizations such that r is in material i. Hence, Eq. (33) becomes

$$\frac{1}{v}\frac{\partial(p_i\psi_i)}{\partial t} + \Omega\cdot\nabla(p_i\psi_i) + \Sigma_{ti}(p_i\psi_i) = \frac{\Sigma_{si}}{4\pi}\int_{4\pi}p_i\psi_i(r,\Omega',t)d\Omega' + \frac{p_iQ_i}{4\pi} + \big\langle\psi(\Omega\cdot\nabla\chi_i)\big\rangle. \tag{36}$$

Further, using Eq. (28) and equations (34) and (35), we deduce that

$$\big\langle\psi(r,\Omega,t)\big\rangle = p_1(r)\psi_1(r,\Omega,t) + p_2(r)\psi_2(r,\Omega,t), \tag{37}$$

which is the overall ensemble average of the angular flux as defined earlier. Boundary and initial conditions for $\psi_i(r,\Omega,t)$ are obtained by multiplying equations (25) and (26) by $\chi_i(r)$ and ensemble-averaging them:

$$\psi_i(r_s,\Omega,t) = \Gamma(r_s,\Omega,t), \quad n\cdot\Omega < 0, \tag{38}$$

$$\psi_i(r,\Omega,0) = \alpha(r,\Omega). \tag{39}$$

Now, to obtain a closed system of equations and boundary conditions for ψ_1 and ψ_2, it is necessary to evaluate the term $\big\langle f_i(r,\Omega,t)\big\rangle = \big\langle\psi(r,\Omega,t)[\Omega\cdot\nabla\chi_i(r)]\big\rangle$ on the right hand side of Eq. (36). To do this, we consider the average value of $f_i(r,\Omega,t)$ over a volume V, and take the limit as V approaches zero:

$$\big\langle f_i(r,\Omega,t)\big\rangle = \lim_{V\to 0}\left\langle\psi(r,\Omega,t)\left(\frac{1}{V}\int_V\Omega\cdot\nabla\chi_i(r)dr\right)\right\rangle. \tag{40}$$

The ensemble-average in Eq. (40) is over all realizations. However, for a given realization, we have $\int_V \Omega \cdot \nabla\chi_i(r)dr \neq 0$ only if there is an interface between materials 1 and 2 intersecting V. Therefore, we write

$$\left\langle \psi(r,\Omega,t)\left(\frac{1}{V}\int_V \Omega\cdot\nabla\chi_i(r)dr\right)\right\rangle = P^*\left\langle \psi(r,\Omega,t)\left(\frac{1}{V}\int_V \Omega\cdot\nabla\chi_i(r)dr\right)\right\rangle^*, \qquad (41)$$

where P^* is the probability that a realization has an interface that intersects V, and $\left\langle\,\cdot\,\right\rangle^*$ is a restricted average, defined to be an ensemble average over all realizations having an interface that intersects V.

Now, we consider V to be a sphere of radius ε centered at r. Assuming that there exists an interface intersecting this sphere, for ε small enough we can regard this interface as a plane with normal vector n_i pointing out of region i. If we chose the z-axis perpendicular to this planar interface as shown in Fig. 3, then the intersection of the interface with the sphere is a

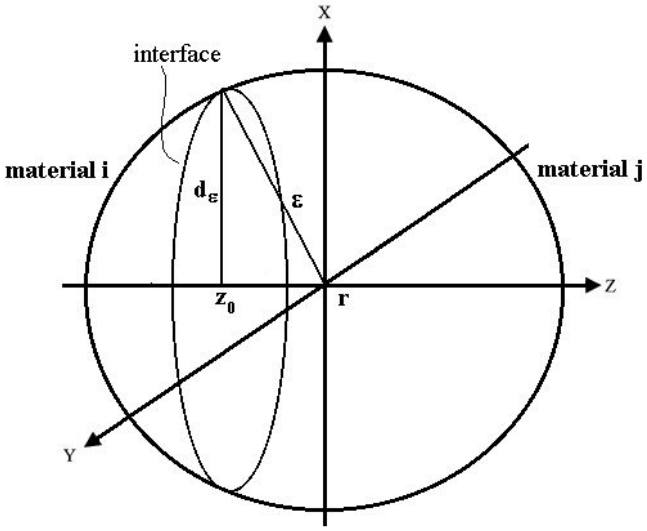

Figure 3: Intersection of the interface with the sphere V

disc of radius $d_\varepsilon = \sqrt{\varepsilon^2 - z_0^2}$, given by the intersection of the plane $z = z_0$ with the sphere, and $n_i = \hat{e}_z$. In this coordinate system, $\nabla\chi(r) = -n_i\delta(z - z_0)$; thus

$$\begin{aligned}\frac{1}{V}\int_V \Omega\cdot\nabla\chi_i(r)dr &= \frac{3}{4\pi\varepsilon^3}\int_V(-\Omega\cdot n_i)\delta(z-z_0)dxdydz = \\ &= \frac{3}{4\pi\varepsilon^3}(-\Omega\cdot n_i)\pi d_\varepsilon^2 = \frac{3}{4\varepsilon^3}(-\Omega\cdot n_i)d_\varepsilon^2,\end{aligned} \qquad (42)$$

and Eq. (40) becomes

$$\left\langle f_i(r,\Omega,t)\right\rangle = \lim_{\varepsilon\to 0}\left[-\frac{3}{4\varepsilon^3}P^*\left\langle(\Omega\cdot n_i)\psi(r,\Omega,t)d_\varepsilon^2\right\rangle^*\right]. \qquad (43)$$

Let us define $\left\langle\,\cdot\,\right\rangle^*_{\Omega\cdot n_i>0}$ to be the ensemble average over all realizations such that an interface intersects V and Ω points out of material i. Then, since $n_i = -n_j$,

$$\begin{aligned}\left\langle (\Omega\cdot n_i)\psi(r,\Omega,t)d_\varepsilon^2\right\rangle^* &= \\ &= \left\langle (\Omega\cdot n_i)\psi(r,\Omega,t)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i>0} + \left\langle (\Omega\cdot n_i)\psi(r,\Omega,t)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i<0} \\ &= \left\langle (\Omega\cdot n_i)\psi(r,\Omega,t)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i>0} - \left\langle (\Omega\cdot n_j)\psi(r,\Omega,t)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_j>0},\end{aligned} \tag{44}$$

and defining

$$\Psi_i^\varepsilon = \frac{\left\langle (\Omega\cdot n_i)\psi(r,\Omega,t)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i>0}}{\left\langle (\Omega\cdot n_i)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i>0}} \tag{45}$$

we can rewrite Eq. (43) as

$$\left\langle f_i(r,\Omega,t)\right\rangle = \lim_{\epsilon\to 0}\left[\frac{3}{4\varepsilon^3}P^*\left(\Psi_j^\varepsilon\left\langle (\Omega\cdot n_j)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_j>0} - \Psi_i^\varepsilon\left\langle (\Omega\cdot n_i)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i>0}\right)\right]. \tag{46}$$

The geometrical quantities $\left\langle (\Omega\cdot n_i)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i>0}$ in Eq. (46) are equal for $i=1,2$, and can be explicitly evaluated if we assume:

1) the points z_0 in Fig. 3 to be uniformly distributed on $-\varepsilon < z_0 < \varepsilon$;
2) the normal vectors of interfaces passing through V to be uniformly distributed on the unit sphere.

Then, using $\Omega\cdot n_i = \mu$ and $d_\varepsilon^2 = \varepsilon^2 - z_0^2$, we obtain for $i=1$ and 2

$$\begin{aligned}\left\langle (\Omega\cdot n_i)d_\varepsilon^2\right\rangle^*_{\Omega\cdot n_i>0} &= \left\langle \mu(\varepsilon^2-z_0^2)\right\rangle^*_{\mu>0} \\ &= \int_0^1\left(\frac{1}{2\varepsilon}\int_{-\varepsilon}^{\varepsilon}\mu(\varepsilon^2-z_0^2)dz_0\right)d\mu \\ &= \frac{\varepsilon^2}{3}.\end{aligned} \tag{47}$$

Introducing this result into Eq. (46), we get

$$\left\langle f_i(r,\Omega,t)\right\rangle = \lim_{\epsilon\to 0}\left[\frac{3}{4\varepsilon^3}\frac{\varepsilon^2}{3}P^*\left(\Psi_j^\varepsilon-\Psi_i^\varepsilon\right)\right] = \lim_{\epsilon\to 0}\left[\frac{1}{4\varepsilon}P^*\left(\Psi_j^\varepsilon-\Psi_i^\varepsilon\right)\right]. \tag{48}$$

Further, it is possible to calculate P^*. To do this, let us consider an arbitrary infinite line through the point r, and let us assume that the interfaces all intersect the line perpendicularly. Then, it can be seen from Fig. 4 that an interface intersects V only if the point r lies within a distance ε of an interface. This creates a line segment of width 2ε about each interface, such that if r is in one of these segments, then an interface intersects V. Over a very large length of this line, spanning n chunks of material i and n chunks of material j, we have

$$\begin{aligned}(2\mathrm{n})(2\varepsilon) &= 4\mathrm{n}\varepsilon \\ &= \begin{pmatrix}\text{the length of the line segments such that if } r \text{ lies on} \\ \text{one of these segments, then an interface intersects } V\end{pmatrix},\end{aligned} \tag{49}$$

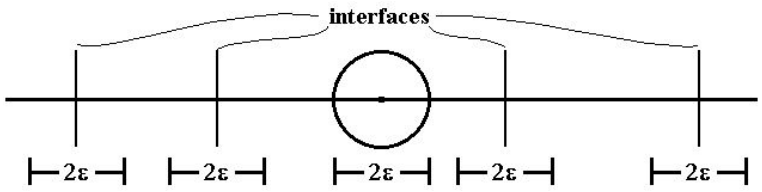

Figure 4: Arbitrary infinite line intersecting interfaces perpendicularly

and

$$\mathrm{n}(\Lambda_1 + \Lambda_2) \approx (\text{total length of the line}). \tag{50}$$

The ratio of equations (49) and (50) is P^*, that is,

$$P^* = \frac{4\varepsilon}{\Lambda_1 + \Lambda_2}, \tag{51}$$

and one can easily see that this expression has the right qualitative behavior. It correctly limits to zero as $\varepsilon \to 0$, and as $\Lambda_1, \Lambda_2 \to \infty$.

Introducing Eq. (51) into Eq. (48), we obtain

$$\left\langle f_i(r,\Omega,t)\right\rangle = \lim_{\epsilon\to 0}\left[\frac{1}{4\varepsilon}\left(\frac{4\varepsilon}{\Lambda_1+\Lambda_2}\right)\left(\Psi_j^\varepsilon - \Psi_i^\varepsilon\right)\right] = \lim_{\epsilon\to 0}\left[\frac{1}{\Lambda_1+\Lambda_2}\left(\Psi_j^\varepsilon - \Psi_i^\varepsilon\right)\right]. \tag{52}$$

Finally, defining $\Psi_i = \lim_{\varepsilon\to 0}\Psi_i^\varepsilon$ and using Eq. (23), we have

$$\begin{aligned}\left\langle f_i(r,\Omega,t)\right\rangle &= \frac{1}{\Lambda_1+\Lambda_2}\left(\Psi_j - \Psi_i\right)\\ &= \frac{p_j\Psi_j}{\Lambda_j} - \frac{p_i\Psi_i}{\Lambda_i},\end{aligned} \tag{53}$$

and this result is the Levermore-Pomraning expression for $\left\langle f_i\right\rangle$. Combining Eq. (36) with Eq. (53), we obtain

$$\frac{1}{v}\frac{\partial(p_i\psi_i)}{\partial t} + \Omega\cdot\nabla(p_i\psi_i) + \Sigma_{ti}(p_i\psi_i) = \frac{\Sigma_{si}}{4\pi}\int_{4\pi} p_i\psi_i(r,\Omega',t)d\Omega' + \frac{p_iQ_i}{4\pi} + \frac{p_j\Psi_j}{\Lambda_j} - \frac{p_i\Psi_i}{\Lambda_i}. \tag{54}$$

Unfortunately, this result consists of two equations with four unknown functions, namely ψ_1, ψ_2, Ψ_1 and Ψ_2; thus, a closure is needed to make this formalism useful. No simple exact relationship seems to exist relating ψ_i (the ensemble average of ψ over all physical realizations such that r is in material i) and Ψ_i (the ensemble average of ψ at interface points for which $\Omega\cdot n_i > 0$). Nevertheless, in analogy with upwind differencing encountered in the numerical analysis of hyperbolic equations, we approximate Ψ_i simply replacing it with ψ_i. This is the "classic" Levermore-Pomraning closure, and using it we rewrite Eq. (54) as

$$\frac{1}{v}\frac{\partial(p_i\psi_i)}{\partial t} + \Omega\cdot\nabla(p_i\psi_i) + \Sigma_{ti}(p_i\psi_i) = \frac{\Sigma_{si}}{4\pi}\int_{4\pi} p_i\psi_i(r,\Omega',t)d\Omega' + \frac{p_iQ_i}{4\pi} + \frac{p_j\psi_j}{\Lambda_j} - \frac{p_i\psi_i}{\Lambda_i}, \tag{55}$$

and the general case (general scattering, arbitrary source) is straightforwardly given by

$$\frac{1}{v}\frac{\partial(p_i\psi_i)}{\partial t} + \Omega\cdot\nabla(p_i\psi_i) + (\Sigma_{ai}+S_i)(p_i\psi_i) = p_iQ_i + \frac{p_j\psi_j}{\Lambda_j} - \frac{p_i\psi_i}{\Lambda_i}, \tag{56}$$

where S_i is the scattering operator defined by

$$S_i\psi_i = \Sigma_{si}\psi_i - \int_0^\infty \int_{4\pi} \Sigma_{si}(r, E' \to E, \Omega' \cdot \Omega, t)\psi_i(r, E', \Omega', t)d\Omega' dE'. \tag{57}$$

The coupled equations ($i = 1, 2$) given by Eq. (56) are known as the "classic" Levermore-Pomraning equations. As a remark, we mention that the atomic mix model can be deduced from the Levermore-Pomraning equations through the use of asymptotic limits (Pomraning, 1991).

These considerations can be easily extended to nonstatic physical realizations of the mixing. In this case, the characteristic functions will also depend upon the time variable, and a new term will appear on the right-hand side of Eq. (33), namely

$$\frac{\psi}{v}\frac{\partial\chi_i(r,t)}{\partial t}. \tag{58}$$

Treating this term in analogy with the way we treated $\langle f_i \rangle$ in the present derivation, one should obtain another pair of Levermore-Pomraning equations, with extra terms representing the time stochasticity.

Finally, it is important to notice that, in general, the assumption that the interfaces all intersect an arbitrary line perpendicularly (Fig. 4) cannot be true. Although it leads to the "classic" Levermore-Pomraning equation, we get a different result when this assumption is not made. We hope to contemplate this issue in future work, in order to improve the present model.

4. NUMERICAL RESULTS

We consider time independent transport in planar geometry without internal sources. In this case, assuming isotropic and coherent scattering, Eq. (1) is written

$$\mu\frac{\partial\psi(z,\mu)}{\partial z} + \Sigma_t(z)\psi(z,\mu) = \frac{\Sigma_s(z)}{2}\int_{-1}^{1}\psi(z,\mu')d\mu', \tag{59}$$

where μ is the cosine of the angle between the z-axis and the particle's direction of travel. We take Eq. (59) to hold on the interval $0 \le z \le Z$, and we consider an isotropic intensity, normalized to a unit incoming flux, incident upon the planar system at $z = 0$; and no intensity incident upon the system at $z = Z$. This corresponds to the boundary conditions

$$\begin{cases} \psi(0,\mu) = 2, & \mu > 0 \\ \psi(Z,\mu) = 0, & \mu < 0 \end{cases}. \tag{60}$$

In analogy with the previous discussion, we take this system to be statistically composed of alternating slabs of two materials, such that each material has spatially independent cross sections Σ_t and Σ_s. The statistics of this situation is assumed to be a homogeneous Markov process, which implies (Pomraning, 1991) that the thickness of each slab of material i is chosen at random from an exponential distribution given by

$$\mathrm{f}_i(\xi) = \Lambda_i^{-1}e^{-\xi/\Lambda_i}. \tag{61}$$

Here, $\mathrm{f}_i(\xi)d\xi$ is the probability of a segment of material i having a length lying between ξ and $\xi + d\xi$, and Λ_i is the mean slab thickness of material i, such that

$$\Lambda_i = \int_0^\infty \xi\mathrm{f}_i(\xi)d\xi. \tag{62}$$

At any point in this system, the probability p_i of finding material i is given by Eq. (23). To obtain ensemble-averaged results for this transport problem, we first generate a physical realization of the statistics using a Monte Carlo procedure, and for this realization we solve the corresponding transport problem. We used the LTS$_N$ formulation for a multi-region slab (Segatto et al., 2001) to obtain this solution, with $N = 50$.

To obtain a physical realization, we first choose the material present at $z = 0$ statistically according to the probabilities p_i. Then, we sample from Eq. (61) for the value of i so determined to establish the length of the first segment of this material, with its left-hand boundary at $z = 0$. We next sample from Eq. (61) with the other material index to determine the length of the next segment. We then sample from Eq. (61) with the original index i to determine the length of the third segment. We continue this process until the entire interval $0 \leq z \leq Z$ is populated with alternating segments of the two materials.

We computed the probabilities of reflection R and transmission T for the system, as given by

$$R = \int_0^1 \mu\psi(0, -\mu)d\mu, \quad T = \int_0^1 \mu\psi(Z, \mu)d\mu. \tag{63}$$

The probability of absorption A follows from particle conservation, such that $A = 1 - R + T$.

Repeating this process for a large number of physical realizations, ensemble-averaged results for the reflection and transmission follow from simple numerical averages, such that

$$\langle R \rangle = \frac{1}{K}\sum_{k=1}^{K} R_k, \quad \langle T \rangle = \frac{1}{K}\sum_{k=1}^{K} T_k. \tag{64}$$

Here, the index k denotes a particular realization of the statistics, and K represents the number of realizations computed. Also, one can calculate the standard deviation σ of these results according to

$$\sigma^2(R) = \left| \langle R \rangle^2 - \frac{1}{K}\sum_{k=1}^{K} R_k^2 \right|, \quad \sigma^2(T) = \left| \langle T \rangle^2 - \frac{1}{K}\sum_{k=1}^{K} T_k^2 \right|, \tag{65}$$

which gives an indication of the spread of the results about the means.

We have used this procedure to obtain results for four different sets of Σ_{ti}, Σ_{si} and Λ_i. These results are given in Tables 1-4 in the "Exact" columns. We also provide in these columns, between parenthesis, the number of realizations computed. It is important to notice that, different from the other cases where K was chosen to be 10^5, we chose $K = 10^4$ in Tables 1 and 3 for the slab thickness $Z = 1.0$. We did this for cpu time reasons, and we believe that the sampling error we get is approximately the same we would obtain if we chose $K = 10^5$, since in these cases each physical realization contains an average of ten regions of each material.

The predictions of the atomic mix and the Levermore-Pomraning models are also displayed in Tables 1-4, numerically calculated using the LTS$_N$ formulation (Segatto et al., 1999; Segatto et al., 2001), with $N = 50$. For the problem under consideration, the atomic mix equations (15) and (16) are written

$$\mu\frac{\partial\langle\psi\rangle}{\partial z} + \langle\Sigma_t\rangle\langle\psi\rangle = \frac{\langle\Sigma_s\rangle}{2}\int_{-1}^{1}\langle\psi(z, \mu')\rangle d\mu', \tag{66}$$

$$\begin{cases} \langle\psi(0, \mu)\rangle = 2, & \mu > 0 \\ \langle\psi(Z, \mu)\rangle = 0, & \mu < 0 \end{cases}, \tag{67}$$

Table 1: Reflection and transmission results

$\Lambda_1 = 0.1$	$\Sigma_{t1} = 0.1$	$\Sigma_{s1} = 0.0$	$\Sigma_{t1}\Lambda_1 = 0.01$
$\Lambda_2 = 0.01$	$\Sigma_{t2} = 2.5$	$\Sigma_{s2} = 2.5$	$\Sigma_{t2}\Lambda_2 = 0.025$

$Z = 0.1$	Exact (10^5)	Atomic Mix	Levermore Pomraning	:	$Z = 1.0$	Exact (10^4)	Atomic Mix	Levermore Pomraning
$< R >$	0.0199	0.0209	0.0198	:	$< R >$	0.1314	0.1346	0.1308
$\sigma(R)$	0.0245	*	*	:	$\sigma(R)$	0.0479	*	*
$< T >$	0.9626	0.9616	0.9627	:	$< T >$	0.7119	0.7077	0.7124
$\sigma(T)$	0.0222	*	*	:	$\sigma(T)$	0.0419	*	*
Time (s)	5581.3	0.28	0.33	:	Time (s)	77702.2	0.01	0.11

Table 2: Reflection and transmission results

$\Lambda_1 = 10.0$	$\Sigma_{t1} = 0.1$	$\Sigma_{s1} = 0.0$	$\Sigma_{t1}\Lambda_1 = 1.0$
$\Lambda_2 = 1.0$	$\Sigma_{t2} = 2.5$	$\Sigma_{s2} = 2.5$	$\Sigma_{t2}\Lambda_2 = 2.5$

$Z = 0.1$	Exact (10^5)	Atomic Mix	Levermore Pomraning	:	$Z = 1.0$	Exact (10^5)	Atomic Mix	Levermore Pomraning
$< R >$	0.0166	0.0209	0.0165	:	$< R >$	0.0737	0.1346	0.0694
$\sigma(R)$	0.0512	*	*	:	$\sigma(R)$	0.1798	*	*
$< T >$	0.9659	0.9616	0.9661	:	$< T >$	0.7738	0.7077	0.7778
$\sigma(T)$	0.0457	*	*	:	$\sigma(T)$	0.1400	*	*
Time (s)	292.7	0.05	0.17	:	Time (s)	503.7	0.05	0.16

where $\langle \Sigma_t \rangle$, $\langle \Sigma_s \rangle$ and $\langle \psi \rangle$ are given in analogy with Eq. (18). Also, the Levermore-Pomraning equations (56) and (38) are written

$$\mu \frac{\partial \psi_i(z,\mu)}{\partial z} + \Sigma_{ti}\psi_i(z,\mu) = \frac{\Sigma_{si}}{2}\int_{-1}^{1} \psi_i(z,\mu')d\mu' + \frac{|\mu|}{\Lambda_i}\big[\psi_j(z,\mu) - \psi_i(z,\mu)\big], \tag{68}$$

$$\begin{cases} \psi_i(0,\mu) = 2, & \mu > 0, \\ \psi_i(Z,\mu) = 0, & \mu < 0, \end{cases}, \tag{69}$$

and the ensemble-averaged solution $\langle \psi \rangle$ is given according to Eq. (37). Here, it is important to explain the term $|\mu|/\Lambda_i$ in Eq. (68). If the mean slab thickness of material i is Λ_i, then the mean chord length seen by a particle traveling at an angle characterized by its cosine μ is just $\Lambda_i/|\mu|$. That is, the mean chord length through material i is angularly dependent, which leads to this form of Eq. (68).

All numerical calculations were performed on a Pentium III 1.0 GHz; the cpu times are displayed (in seconds) at the bottom of Tables 1-4. Our goal in presenting these results is to compare the atomic mix and the Levermore-Pomraning models, and to test their accuracy.

As expected, the atomic mix model presents itself better when $Z = 0.1$. We can see from Tables 1 and 3 that its results are quite accurate when the product $\Sigma_{ti}\Lambda_i$ approaches zero. In fact, examining its relative error given by

$$\text{Relative Error (\%)} = 100\frac{|\text{Exact} - \text{Atomic Mix}|}{\text{Exact}}, \tag{70}$$

we will find it to be smaller than 7% in these Tables.

Table 3: Reflection and transmission results

$\Lambda_1 = 0.1$	$\Sigma_{t1} = 0.1$	$\Sigma_{s1} = 0.1$	$\Sigma_{t1}\Lambda_1 = 0.01$
$\Lambda_2 = 0.01$	$\Sigma_{t2} = 2.5$	$\Sigma_{s2} = 0.0$	$\Sigma_{t2}\Lambda_2 = 0.025$

$Z = 0.1$	Exact (10^5)	Atomic Mix	Levermore Pomraning	:	$Z = 1.0$	Exact (10^4)	Atomic Mix	Levermore Pomraning
$< R >$	0.0084	0.0081	0.0083	:	$< R >$	0.0487	0.0453	0.0476
$\sigma(R)$	0.0017	*	*	:	$\sigma(R)$	0.0116	*	*
$< T >$	0.9512	0.9489	0.9513	:	$< T >$	0.6353	0.6247	0.6342
$\sigma(T)$	0.0480	*	*	:	$\sigma(T)$	0.0927	*	*
Time (s)	5113.1	0.01	0.12	:	Time (s)	71299.3	0.01	0.11

Table 4: Reflection and transmission results

$\Lambda_1 = 10.0$	$\Sigma_{t1} = 0.1$	$\Sigma_{s1} = 0.1$	$\Sigma_{t1}\Lambda_1 = 1.0$
$\Lambda_2 = 1.0$	$\Sigma_{t2} = 2.5$	$\Sigma_{s2} = 0.0$	$\Sigma_{t2}\Lambda_2 = 2.5$

$Z = 0.1$	Exact (10^5)	Atomic Mix	Levermore Pomraning	:	$Z = 1.0$	Exact (10^5)	Atomic Mix	Levermore Pomraning
$< R >$	0.0089	0.0081	0.0089	:	$< R >$	0.0740	0.0453	0.0727
$\sigma(R)$	0.0028	*	*	:	$\sigma(R)$	0.0255	*	*
$< T >$	0.9591	0.9489	0.9592	:	$< T >$	0.7994	0.6247	0.7997
$\sigma(T)$	0.0970	*	*	:	$\sigma(T)$	0.2712	*	*
Time (s)	296.1	0.01	0.11	:	Time (s)	497.3	0.06	0.11

However, we see that increasing the values of Λ_1 and Λ_2 by the same factor, the atomic mix results remain unchanged and the accuracy of the model deteriorates. This is not unexpected, since in this case the products $\Sigma_{ti}\Lambda_i$ do not satisfy Eq. (13). Indeed, its relative error reaches 82% in Table 2 and 38% in Table 4.

On the other hand, the Levermore-Pomraning model maintain a reasonable order of accuracy when the values of Λ_i increase. Its relative error, calculated in analogy with Eq. (70), is smaller than 6% in all Tables. It is also important to point out that, as observed by Adams et al. (1989), the Levermore-Pomraning model in general underestimate the ensemble-averaged reflection probability $\langle R \rangle$, and overestimate the ensemble-averaged transmission probability $\langle T \rangle$.

Analysing the results reported here, we underline the relevance of developing error estimates for both models presented in this paper. To our knowledge, there are few papers where this subject is considered. We focus our future attention in this direction.

Acknowledgements

Richard Vasques and Marco T. Vilhena are gratefully indebted to CNPq (Conselho Nacional de Desenvolvimento Tecnológico e Científico) for the partial financial support of this work.

REFERENCES

Adams, M. L., Larsen, E. W., & Pomraning, G. C., 1989. Benchmark results for particle transport in a binary markov statistical medium. *Journal of Quantitative Spectroscopy and*

Radiative Transfer, vol. 42, n. 4, pp. 253–266.

Frisch, U., 1968. Wave propagation in random media. In *Probabilistic Methods in Applied Mathematics*, vol. 1, pp. 75–198. Academic Press.

Larsen, E. W., 2003. Asymptotic derivation of the atomic-mix diffusion model for 1-D random diffusive media. In *Proceedings - 18^{th} International Conference on Transport Theory (ICTT)*, pp. 129–132.

Levermore, C. D., Pomraning, G. C., Sanzo, D. L., & Wong, J., 1986. Linear transport theory in a random medium. *Journal of Mathematical Physics*, vol. 27, n. 10, pp. 2526–2536.

Morrison, J. A., 1972. Moments and correlation-functions of solutions of some stochastic matrix differential equations. *Journal of Mathematical Physics*, vol. 13, n. 3, pp. 299–306.

Parzan, E., 1962. *Stochastic Processes.* Wiley-New York.

Pomraning, G. C., 1986. Transport and diffusion in a statistical medium. *Transport Theory and Statistical Physics*, vol. 15, pp. 773–802.

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

Segatto, C. F., Vilhena, M. T., & Gomes, M. G., 1999. The one-dimensional LTS$_N$ solution in a slab with high degree of quadrature. *Annals of Nuclear Energy*, vol. 26, pp. 925–934.

Segatto, C. F., Vilhena, M. T., & Tavares, L. S. S., 2001. The determination of radiant parameters by the LTS$_N$ method. *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 70, pp. 227–236.

Vanderhaegen, D., 1986. Radiative transfer in statistically heterogeneous mixtures. *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 36, pp. 557–561.

Van Kampen, N. G., 1981. *Stochastic Processes in Physics and Chemistry.* North Holland.