NE 255, Fa16
Transport in Stochastic Mixtures
November 29, 2016

These notes are derived from the course "Advanced Topics in Transport Theory", taught at RWTH Aachen University, Germany, on the Summer of 2013.

The Atomic Mix Model (empirical motivation)

Let us consider the integro-differential transport equation. In a deterministic medium, the total cross section Σ_t, the scattering kernel Σ_s, and the source Q are known prescribed functions of their arguments. Thus, in order to find an expression for the angular flux ψ, one must solve this equation subject to the boundary and initial conditions.

Now we consider neutron transport in a heterogeneous volume V such that the boundary ∂V of V is specified, but the interior structure of V is not. 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 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 Figure 1.

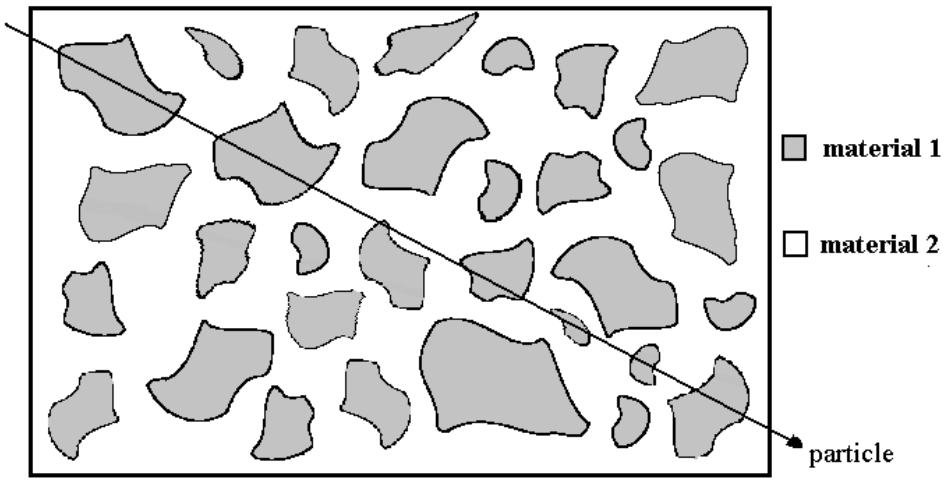

Figure 1: Particle traversing the mixture along a random path

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 $\Sigma_{ti}(\boldsymbol{x}, E, t)$, $\Sigma_{si}(\boldsymbol{x}, E' \to E, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, t)$, and $Q_i(\boldsymbol{x}, E, \boldsymbol{\Omega}, t)$. The stochasticity of the problem is that we have only a probabilistic idea about which material occupies the space point $\boldsymbol{x}$ at a time t. Therefore, since we are considering Σ_t, Σ_s, and Q as random variables, we must also consider the angular flux ψ as a random variable. We want to find an expression for $\langle\psi\rangle$, the ensemble-averaged angular flux (expected value) of ψ.

For convenience, let us consider the case of transport in a non-scattering (i.e. purely absorbing) medium. Thinking about $\boldsymbol{\Omega} \cdot \nabla$ as a directional derivative, we can rewrite the time-dependent transport equation as

$$\frac{1}{v}\frac{\partial\psi(u,t)}{\partial t} + \frac{\partial\psi(u,t)}{\partial u} + \Sigma_t(u,t)\psi(u,t) = Q(u,t), \tag{1}$$

where u denotes the spatial variable in the direction $\boldsymbol{\Omega}$. One must notice that Eq. (1) describes particle transport at each energy E and direction $\boldsymbol{\Omega}$, which are omitted since they are only parameters. We let $\langle W\rangle$ denote 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 Eq. (1) to obtain

$$\frac{1}{v}\frac{\partial\langle\psi\rangle}{\partial t} + \frac{\partial\langle\psi\rangle}{\partial u} + \langle\Sigma_t\rangle\langle\psi\rangle + \langle\tilde{\Sigma}_t\tilde{\psi}\rangle = \langle Q\rangle. \tag{2}$$

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

$$p_1(u,t) + p_2(u,t) = 1, \tag{3}$$

and we can write

$$\langle\Sigma_t(u,t)\rangle = p_1(u,t)\Sigma_{t1}(u,t) + p_2(u,t)\Sigma_{t2}(u,t), \tag{4}$$

$$\langle Q(u,t)\rangle = p_1(u,t)Q_1(u,t) + p_2(u,t)Q_2(u,t). \tag{5}$$

If we write the characteristic chord length (mean chord length) for the chunks of material i as Λ_i and assume that

$$\Sigma_{ti}\Lambda_i \ll 1, \quad i = 1, 2, \tag{6}$$

then a particle between collisions is likely to travel a distance that spans many chunks of materials 1 and 2. This means that Λ_i is very small when compared with the mean free path $\langle s\rangle$. 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.

When Eq. (6) is satisfied, it is physically intuitive that the transport process will be well-approximated by the process that holds when the chunk sizes are zero in the limit (the atomic mix limit). Moreover, when the chunk sizes shrink, the deviations in the angular flux should also shrink, and $\tilde{\psi}$ will go to zero. Hence, the cross correlation term $\langle \tilde{\Sigma}_t \tilde{\psi} \rangle$ in Eq. (2) can be safely neglected, and Eq. (2) becomes

$$\frac{1}{v}\frac{\partial \langle \psi \rangle}{\partial t} + \frac{\partial \langle \psi \rangle}{\partial u} + \langle \Sigma_t \rangle \langle \psi \rangle = \langle Q \rangle, \tag{7}$$

which is closed for the ensemble-averaged angular flux $\langle \psi \rangle$. This equation represents the atomic mix description of Eq. (1).

Applying the same arguments on the general form of the transport equation, the atomic mix description of stochastic transport, including scattering, is given by

$$\begin{aligned} &\frac{1}{v}\frac{\partial \langle \psi(\boldsymbol{x}, E, \boldsymbol{\Omega}, t) \rangle}{\partial t} + \boldsymbol{\Omega} \cdot \nabla \langle \psi(\boldsymbol{x}, E, \boldsymbol{\Omega}, t) \rangle + \langle \Sigma_t(\boldsymbol{x}, E, t) \rangle \langle \psi(\boldsymbol{x}, E, \boldsymbol{\Omega}, t) \rangle = \\ &\quad = \int_0^\infty \int_{4\pi} \langle \Sigma_s(\boldsymbol{x}, E' \to E, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, t) \rangle \langle \psi(\boldsymbol{x}, E', \boldsymbol{\Omega}', t) \rangle d\Omega' dE' + \langle Q(\boldsymbol{x}, E, \boldsymbol{\Omega}, t) \rangle, \end{aligned} \tag{8}$$

with

$$\langle \psi(\boldsymbol{x}_s, E, \boldsymbol{\Omega}, t) \rangle = \langle \psi_s(\boldsymbol{x}_s, E, \boldsymbol{\Omega}, t) \rangle, \quad \mathbf{n} \cdot \boldsymbol{\Omega} < 0, \tag{9}$$

$$\langle \psi(\boldsymbol{x}, E, \boldsymbol{\Omega}, 0) \rangle = \langle \psi_0(\boldsymbol{x}, E, \boldsymbol{\Omega}) \rangle. \tag{10}$$

Here

$$\langle W \rangle = p_1(\boldsymbol{x}, t) W_1 + p_2(\boldsymbol{x}, t) W_2, \tag{11}$$

where W stands for Σ_t, Σ_s, and Q. The neglected cross correlation terms are $\langle \tilde{\Sigma}_t \tilde{\psi} \rangle$ and $\langle \tilde{\Sigma}_s \tilde{\psi} \rangle$.

The Multiscale Expansion Technique for Deriving Atomic Mix

So far we have discussed only an empirical way to obtain the atomic mix equation. Now, we will derive a simplified version of the atomic mix equationus ing the formal procedure of multiscale expansions, following the idea presented by Dumas and Golse [1]. (For those interested, the cited paper contains a rigorous derivation of the method, proving that the atomic mix approximation is an asymptotic limit of the particle transport equation as the chunk widths of the materials limit to zero.)

Let us consider time independent transport in a 3-D volume in which heterogeneities occur along one spatial dimension (x) only. Moreover, let this volume consist of binary walls placed perpen-

dicularly to the x-axis. A transverse intersection of this volume is represented by the multilayered slab in Figure 2, where Λ_i is the mean width of the regions of the homogeneous material i

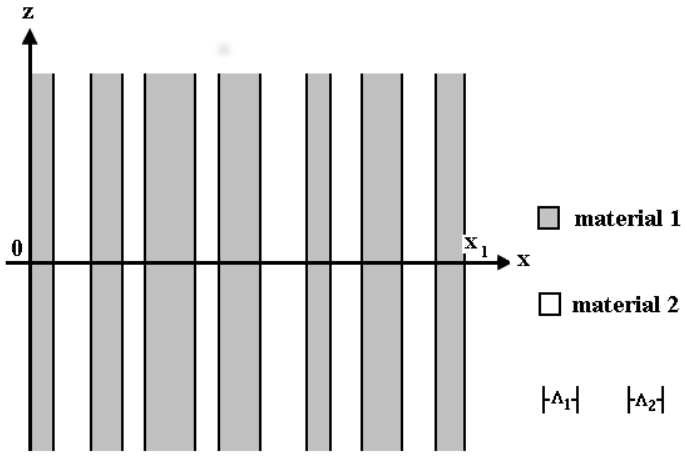

Figure 2: Multilayered slab - transverse volume intersection

($i = 1, 2$).

Denoting the mean free path of a particle in this system as by $\langle s \rangle$, we define

$$\Lambda = \frac{\Lambda_1 + \Lambda_2}{2}, \tag{12}$$

and assuming that Eq. (6) holds, which characterizes a mixture at atomic level, we define the small parameter ε by

$$\frac{\Lambda}{\langle s \rangle} = \varepsilon \ll 1. \tag{13}$$

For simplicity, we will assume that the scattering process is both coherent and isotropic, and that the source Q emmits particles isotropically. It is therefore clear that Σ_t, Σ_s, and Q will depend only upon the spatial variable x, since our assumptions allow us to consider energy E as a simple parameter. In this case, the steady-state transport equation is given by

$$\boldsymbol{\Omega} \cdot \nabla \psi(\boldsymbol{x}, \boldsymbol{\Omega}) + \Sigma_t(x)\psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \frac{\Sigma_s(x)\phi(\boldsymbol{x})}{4\pi} + \frac{Q(x)}{4\pi}, \tag{14}$$

where ϕ is the scalar flux. The (vacuum) boundary condition is given by

$$\psi(\boldsymbol{x}_s, \boldsymbol{\Omega}) = 0, \quad \mathbf{n} \cdot \boldsymbol{\Omega} < 0, \tag{15}$$

where $\boldsymbol{x}_s$ is a point on the surface and $\mathbf{n}$ is a unit outward normal vector at this point.

One must notice that the smaller is ε, the faster will be the oscillations of the functions Σ_t, Σ_s, and Q. This corresponds to the different values of these functions in each component of the mixture. For this reason, a scaling variable $w = x/\varepsilon$ is introduced [1, 2, 3], and we define

$$\Sigma_t(x) = \sigma_t(w), \tag{16a}$$

$$\Sigma_s(x) = \sigma_s(w), \tag{16b}$$

$$Q(x) = q(w), \tag{16c}$$

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}) = \hat{\psi}(\boldsymbol{x}, w, \boldsymbol{\Omega}). \tag{16d}$$

Clearly, this "fast" spatial variable w describes variations in the cross sections, source, and angular flux that occur over distances (along the x-axis) that are small compared to a mean free path. Rewriting Eq. (14) in terms of this scaling variable, we find

$$\boldsymbol{\Omega} \cdot \nabla_w \hat{\psi}(\boldsymbol{x}, w, \boldsymbol{\Omega}) + \boldsymbol{\Omega} \cdot \nabla \hat{\psi}(\boldsymbol{x}, w, \boldsymbol{\Omega}) + \sigma_t(w)\hat{\psi}(\boldsymbol{x}, w, \boldsymbol{\Omega}) = \frac{\sigma_s(w)\hat{\phi}(\boldsymbol{x}, w)}{4\pi} + \frac{q(w)}{4\pi}, \tag{17}$$

that is,

$$\frac{\mu}{\varepsilon}\frac{\partial \hat{\psi}}{\partial w}(\boldsymbol{x}, w, \boldsymbol{\Omega}) + \boldsymbol{\Omega} \cdot \nabla \hat{\psi}(\boldsymbol{x}, w, \boldsymbol{\Omega}) + \sigma_t(w)\hat{\psi}(\boldsymbol{x}, w, \boldsymbol{\Omega}) = \frac{\sigma_s(w)\hat{\phi}(\boldsymbol{x}, w)}{4\pi} + \frac{q(w)}{4\pi}, \tag{18}$$

where $\hat{\phi}$ follows the scalar flux definition regarding $\hat{\psi}$.

Then, we seek $\hat{\psi}$ as a multiscale expansion of the form

$$\hat{\psi}(\boldsymbol{x}, w, \boldsymbol{\Omega}) = \sum_{k=0} \varepsilon^k \psi_k(\boldsymbol{x}, w, \boldsymbol{\Omega}). \tag{19}$$

Proceeding as in [1], we apply this expansion in Eq. (18), and equating the coefficients of powers ε^{-1} and ε^0, we respectively obtain

$$\mu \frac{\partial \psi_0}{\partial w}(\boldsymbol{x}, w, \boldsymbol{\Omega}) = 0, \tag{20}$$

and

$$\mu \frac{\partial \psi_1}{\partial w}(\boldsymbol{x}, w, \boldsymbol{\Omega}) = -\boldsymbol{\Omega} \cdot \nabla \psi_0(\boldsymbol{x}, w, \boldsymbol{\Omega}) - \sigma_t(w)\psi_0(\boldsymbol{x}, w, \boldsymbol{\Omega}) + \frac{\sigma_s(w)\phi_0(\boldsymbol{x}, w)}{4\pi} + \frac{q(w)}{4\pi}, \tag{21}$$

where ϕ_0 follows the scalar flux definition regarding ψ_0. From Eq. (20) we deduce that ψ_0 (and

ϕ_0) does not depend on w. If we define a fast spatial averaging operator [2, 3] by

$$\overline{f}(\boldsymbol{x}) = \lim_{\hat{w}\to\infty}\left[\frac{1}{2\hat{w}}\int_{-\hat{w}}^{\hat{w}} f(\boldsymbol{x},w)dw\right], \tag{22}$$

it is easy to see that

$$\overline{\frac{\partial\psi_1}{\partial w}} \to 0. \tag{23}$$

Hence, applying this operator in Eq. (21), we obtain

$$\boldsymbol{\Omega}\cdot\nabla\psi_0(\boldsymbol{x},\boldsymbol{\Omega}) + \overline{\sigma_t}\;\psi_0(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{\overline{\sigma_s}\;\phi_0(\boldsymbol{x})}{4\pi} + \frac{\overline{q}}{4\pi}, \tag{24}$$

which is the atomic mix representation of Eq. (14). Notice that the averaged quantities obtained with the operator described in Eq. (22) are written throughout these notes with the ensemble-averaging notation $\left\langle\,\cdot\,\right\rangle$.

This derivation presents a simple approach to deal with the heterogeneities of the system. One can think of the neglected cross correlation terms mentioned in the last section as being embodied in the evaluation of the subsequent terms of the expansion in Eq. (19); that is, one can envision that the cross correlation terms must be embodied in $\psi' = \hat{\psi} - \psi_0$.

Atomic mix is very appealing because of its simplicity. Since the cross correlation terms are neglected, this model leads to a description that essentially does not deal with stochastic effects. Assuming that the statistics of mixing is known, the problem of solving Eq. (8) is not different than the one we face to solve the homogeneous transport equation. However, when Eq. (6) is not satisfied, the atomic mix description is generally inaccurate. Although there exist specified classes of problems in which atomic mix is accurate even when the chunk sizes are not optically small [2, 3], 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

$$\frac{\partial\psi(u)}{\partial u} + \Sigma_t(u)\psi(u) = 0, \tag{25}$$

with the boundary condition

$$\psi(0) = \psi_s, \tag{26}$$

where ($0 \le u < \infty$). Let material 1 be composed of optically thin packets such that $\Sigma_{t1}\Lambda_1 \ll 1$. Then, define material 2 as very sparse optically thick chunks imbedded on material 1, in such way that $\Sigma_{t2}\Lambda_2 \gg 1$ and $p_2(u) \ll 1$. Here, Λ_i is the characteristic chord length of material i and p_2 is the probability of finding material 2 at position u. The physical description is that of a near

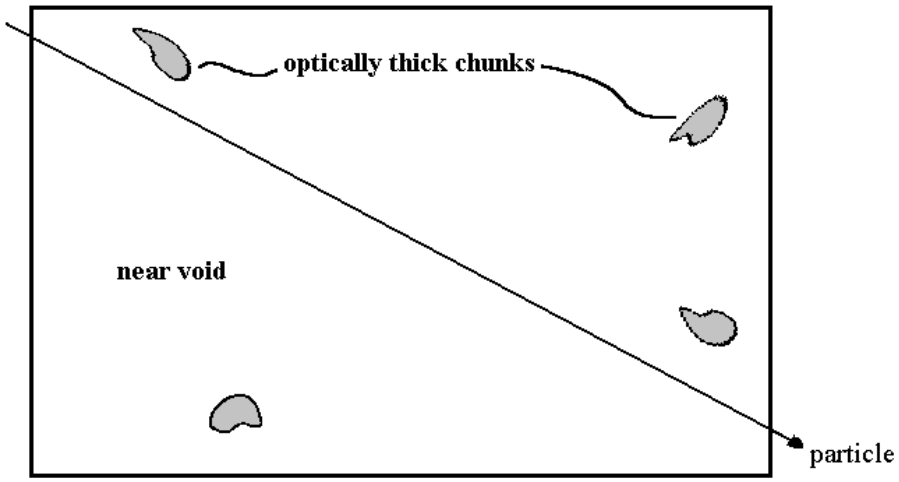

Figure 3: Particle travelling through a near void with sparse chunks

vacuum where sparse absorbing packets of (essentialy) infinite optical thickness can be found. Particles traveling through this mixture tend to pass through it without undergoing an interaction, at least on the average, as can be seen from Figure 3. On the other hand, if we write the atomic mix description of Eqs. (25-26) neglecting the cross correlation term $\langle \tilde{\Sigma}_t \tilde{\psi} \rangle$:

$$\frac{\partial \langle \psi \rangle}{\partial u} + \langle \Sigma_t \rangle \langle \psi \rangle = 0, \tag{27}$$

$$\langle \psi(0) \rangle = \langle \psi_s \rangle, \tag{28}$$

we will conclude that $\langle \psi \rangle$ will be exponentially attenuated, with a scale length $1/\langle \Sigma_t \rangle$, and it is clear that $\langle \Sigma_t \rangle$ is very large, since Σ_{t2} is very large. Hence, this modeling will lead to essentialy no transmission through the system. In general, neglecting the cross correlation term will underestimate particle transmission.

The Levermore-Pomraning Equations

Following Adams, Larsen, and Pomraning [4] and Vasques et al. [5], let us assume a binary stochastic medium whose mixing statistics are arbitrary and known. Also, for simplicity of exposition, we will consider only monoenergetic transport and isotropic scattering.

$$\begin{aligned} \frac{1}{v}\frac{\partial \psi}{\partial t}(\boldsymbol{x}, \boldsymbol{\Omega}, t) + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi(\boldsymbol{x}, \boldsymbol{\Omega}, t) + \Sigma_t(\boldsymbol{x}, t)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, t) = \\ = \frac{\Sigma_s(\boldsymbol{x}, t)}{4\pi} \int_{4\pi} \psi(\boldsymbol{x}, \boldsymbol{\Omega}', t) d\Omega' + Q(\boldsymbol{x}, \boldsymbol{\Omega}, t). \end{aligned} \tag{29}$$

If we introduce the characteristic functions

$$\chi_i(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \boldsymbol{x} \text{ is in material } i \\ 0, & \text{if } \boldsymbol{x} \text{ is in material } j \neq i \end{cases}, \quad i,j \in \{1,2\}, \tag{30}$$

the basic issue is that we do not know the functions $\chi_1(\boldsymbol{x})$ and $\chi_2(\boldsymbol{x})$, but we know that they satisfy

$$\chi_1(\boldsymbol{x}) + \chi_2(\boldsymbol{x}) = 1. \tag{31}$$

(In the following discussion, the $\boldsymbol{x}$ and t dependences are dropped for notational simplicity when convenient.)

Multiplying Eq. (29) by $\chi_i(\boldsymbol{x})$, we can use

$$\chi_i\big[\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{\Omega})\big] = \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i\psi(\boldsymbol{\Omega}) - \psi(\boldsymbol{\Omega})[\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i], \tag{32a}$$

$$\chi_i\Sigma_t = \Sigma_{ti}\chi_i, \tag{32b}$$

$$\chi_i\Sigma_s = \Sigma_{si}\chi_i, \tag{32c}$$

$$\chi_i Q(\boldsymbol{\Omega}) = Q_i(\boldsymbol{\Omega})\chi_i, \tag{32d}$$

to attain

$$\begin{aligned} \frac{1}{v}\frac{\partial\chi_i\psi(\boldsymbol{\Omega})}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i\psi(\boldsymbol{\Omega}) + \Sigma_{ti}\chi_i\psi(\boldsymbol{\Omega}) = \\ = \frac{\Sigma_{si}}{4\pi}\int_{4\pi}\chi_i\psi(\boldsymbol{\Omega}')d\Omega' + Q_i(\boldsymbol{\Omega})\chi_i + \psi(\boldsymbol{\Omega})[\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i]. \end{aligned} \tag{33}$$

Defining $\langle\,\cdot\,\rangle$ as the ensemble average operator over all statistical realizations, the probability of finding material i at position $\boldsymbol{x}$ is given by

$$p_i = \langle\chi_i\rangle, \tag{34a}$$

and therefore we define

$$\psi_i(\boldsymbol{\Omega}) = \frac{\langle\chi_i\psi(\boldsymbol{\Omega})\rangle}{\langle\chi_i\rangle}, \tag{34b}$$

where ψ_i is the ensemble average of $\psi(\boldsymbol{x},\boldsymbol{\Omega},t)$ over all physical realizations such that $\boldsymbol{x}$ is in

material i. By ensemble averaging Eq. (33), we obtain

$$\begin{aligned}\frac{1}{v}\frac{\partial[p_i\psi_i(\boldsymbol{\Omega})]}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}[p_i\psi_i(\boldsymbol{\Omega})] + \Sigma_{ti}[p_i\psi_i(\boldsymbol{\Omega})] = \\ = \frac{\Sigma_{si}}{4\pi}\int_{4\pi}[p_i\psi_i(\boldsymbol{\Omega}')]d\Omega' + p_iQ_i(\boldsymbol{\Omega}) + \big\langle\psi(\boldsymbol{\Omega})[\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i]\big\rangle.\end{aligned} \tag{35}$$

Further, from Eqs. (31) and (34) we deduce that

$$\big\langle\psi(\boldsymbol{\Omega})\big\rangle = p_1\psi_1(\boldsymbol{\Omega}) + p_2\psi_2(\boldsymbol{\Omega}), \tag{36}$$

which is the overall ensemble average of the angular flux.

To evaluate the term $\big\langle f_i(\boldsymbol{x},\boldsymbol{\Omega},t)\big\rangle = \big\langle\psi(\boldsymbol{x},\boldsymbol{\Omega},t)[\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i(\boldsymbol{x})]\big\rangle$ on the right hand side of Eq. (35), we consider the average value of $f_i(\boldsymbol{x},\boldsymbol{\Omega},t)$ over a volume V and take the limit as V approaches zero. This yields

$$\big\langle f_i(\boldsymbol{x},\boldsymbol{\Omega},t)\big\rangle = \lim_{V\to 0}\left\langle\psi(\boldsymbol{x},\boldsymbol{\Omega},t)\left(\frac{1}{V}\int_V\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i(\boldsymbol{x})dV\right)\right\rangle. \tag{37}$$

The ensemble average in Eq. (37) is over all realizations. However, for a given realization, we have $\int_V\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i(\boldsymbol{x})dV \neq 0$ only if there is an interface between materials i and j intersecting V. Therefore, we write

$$\left\langle\psi(\boldsymbol{\Omega})\left(\frac{1}{V}\int_V\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i dV\right)\right\rangle = P^*\left\langle\psi(\boldsymbol{\Omega})\left(\frac{1}{V}\int_V\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i dV\right)\right\rangle^*, \tag{38}$$

where P^* is the probability that a realization has an interface that intersects V, and $\big\langle\ \cdot\ \big\rangle^*$ 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 position $\boldsymbol{x}$ at time t. Assuming that there exists an interface intersecting this sphere, for ε small enough we can regard this interface as a plane with normal vector $\boldsymbol{n_i}$ pointing out of region i. If we chose the x-axis perpendicular to this planar interface (as shown in Figure 4), then the intersection of the interface with the sphere is a disc of radius $d_\varepsilon = \sqrt{\varepsilon^2 - x_0^2}$ given by the intersection of the plane $x = x_0$ with the sphere, and $\boldsymbol{n_i} = \hat{\boldsymbol{e_x}}$. In this coordinate system we have $\boldsymbol{\nabla}\chi(\boldsymbol{x}) = -\boldsymbol{n_i}\delta(x - x_0)$; thus

$$\frac{1}{V}\int_V\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\chi_i(\boldsymbol{x})dV = \frac{3}{4\pi\varepsilon^3}\int_V[-\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]\delta(x - x_0)dxdydz = \frac{3}{4\varepsilon^3}[-\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]d_\varepsilon^2, \tag{39}$$

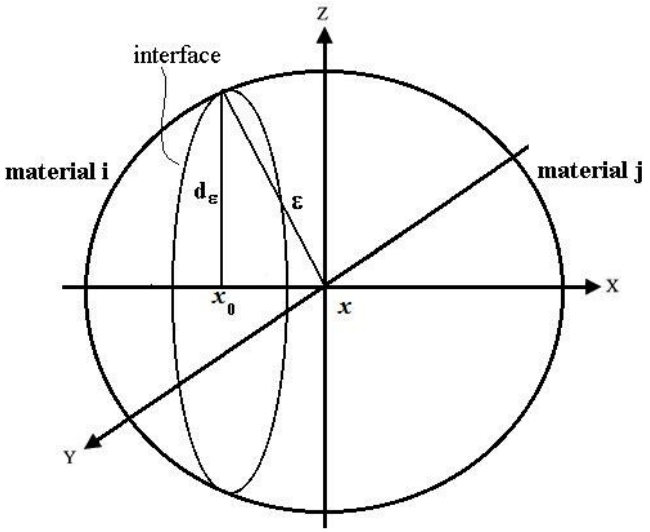

Figure 4: Intersection of the interface with the sphere V

and Eq. (37) becomes

$$\left\langle f_i(\boldsymbol{x},\boldsymbol{\Omega},t)\right\rangle = \lim_{\varepsilon\to 0}\left[-\frac{3}{4\varepsilon^3}P^*\left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d_\varepsilon^2\right\rangle^*\right]. \tag{40}$$

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

$$\begin{aligned}\left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d_\varepsilon^2\right\rangle^* &= \\ &= \left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d_\varepsilon^2\right\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0} + \left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d_\varepsilon^2\right\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}<0} \\ &= \left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d_\varepsilon^2\right\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0} - \left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_j}]\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d_\varepsilon^2\right\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_j}>0}.\end{aligned} \tag{41}$$

Defining

$$\Psi_i^\varepsilon(\boldsymbol{x},\boldsymbol{\Omega},t) = \frac{\left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]\psi(\boldsymbol{x},\boldsymbol{\Omega},t)d_\varepsilon^2\right\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0}}{\left\langle [\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]d_\varepsilon^2\right\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0}} \tag{42a}$$

and

$$\Psi_i(\boldsymbol{x},\boldsymbol{\Omega},t) = \lim_{\varepsilon\to 0}\Psi_i^\varepsilon(\boldsymbol{x},\boldsymbol{\Omega},t), \tag{42b}$$

we can rewrite Eq. (40) as

$$\begin{aligned}\big\langle f_i(\boldsymbol{\Omega})\big\rangle &= \\ &= \lim_{\epsilon\to 0}\left[\frac{3}{4\varepsilon^3}P^*\left(\Psi_j^{\varepsilon}\big\langle[\boldsymbol{\Omega}\cdot\boldsymbol{n_j}]d_{\varepsilon}^2\big\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_j}>0} - \Psi_i^{\varepsilon}\big\langle[\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]d_{\varepsilon}^2\big\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0}\right)\right] \\ &= [\Psi_j(\boldsymbol{\Omega})-\Psi_i(\boldsymbol{\Omega})]\lim_{\epsilon\to 0}\left[\frac{3}{4\varepsilon^3}P^*\big\langle[\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]d_{\varepsilon}^2\big\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0}\right],\end{aligned} \tag{43}$$

since the geometrical quantities $\big\langle[\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]d_{\varepsilon}^2\big\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0}$ are equal for $i\in\{1,2\}$. We point out that Eq. (43) is exact; in fact, with this choice of coordinates, the limit in the equation above is the same geometric quantity dependent upon the statistics that appears in [4] (we will see this next).

We can now rewrite Eq. (35) exactly as

$$\begin{aligned}\frac{1}{v}\frac{\partial[p_i\psi_i(\boldsymbol{\Omega})]}{\partial t} &+ \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}[p_i\psi_i(\boldsymbol{\Omega})] + \Sigma_{ti}[p_i\psi_i(\boldsymbol{\Omega})] = \\ &= \frac{\Sigma_{si}}{4\pi}\int_{4\pi}[p_i\psi_i(\boldsymbol{\Omega}')]d\Omega' + p_iQ_i(\boldsymbol{\Omega}) + \\ &\qquad + [\Psi_j(\boldsymbol{\Omega})-\Psi_i(\boldsymbol{\Omega})]\lim_{\epsilon\to 0}\left[\frac{3}{4\varepsilon^3}P^*\big\langle[\boldsymbol{\Omega}\cdot\boldsymbol{n_i}]d_{\varepsilon}^2\big\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0}\right].\end{aligned} \tag{44}$$

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 $\boldsymbol{x}$ is in material i at time t) and Ψ_i (the ensemble average of ψ at interface points for which $\boldsymbol{\Omega}\cdot\boldsymbol{n_i} > 0$). Nevertheless, Ψ_i can be approximated by simply equating it to ψ_i, in analogy with upwind differencing encountered in the numerical analysis of hyperbolic equations. With this closure, one obtains the LP equations for arbitrary statistics as introduced in [4]. It is important to point out that, in the case of time independent, purely absorbing Markovian media, equating $\Psi_i = \psi_i$ is not an approximation, but an exact identity.

Let us assume that the statistics of the medium is homogeneous. In particular, we assume that

1) the points x_0 in the Figure 4 are uniformly distributed on $-\varepsilon < x_0 < \varepsilon$;
2) the normal vectors of interfaces passing through V are uniformly distributed on the unit sphere.

Then, using $\boldsymbol{\Omega} \cdot \boldsymbol{n_i} = \mu$ and $d_\varepsilon^2 = \varepsilon^2 - x_0^2$, we obtain

$$\begin{aligned} \left\langle (\boldsymbol{\Omega} \cdot \boldsymbol{n_i}) d_\varepsilon^2 \right\rangle^*_{\boldsymbol{\Omega}\cdot\boldsymbol{n_i}>0} &= \left\langle \mu(\varepsilon^2 - x_0^2) \right\rangle^*_{\mu>0} \\ &= \int_0^1 \left(\frac{1}{2\varepsilon} \int_{-\varepsilon}^{\varepsilon} \mu(\varepsilon^2 - x_0^2) dx_0 \right) d\mu \\ &= \frac{\varepsilon^2}{3}. \end{aligned} \tag{45}$$

Introducing this result into Eq. (43), we get

$$\left\langle f_i(\boldsymbol{\Omega}) \right\rangle = [\Psi_j(\boldsymbol{\Omega}) - \Psi_i(\boldsymbol{\Omega})] \lim_{\epsilon \to 0} \left[\frac{1}{4\varepsilon} P^* \right]. \tag{46}$$

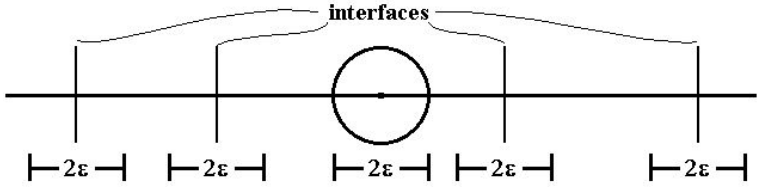

Figure 5: Arbitrary infinite line intersecting interfaces perpendicularly

It is also possible to approximate P^*. To do this, let us consider an arbitrary infinite line through the point $\boldsymbol{x}$, and let us assume it to be the travel path of the particle in the system. Then, it can be seen from Figure 5 that an interface intersects the pathline within V only if the point $\boldsymbol{x}$ lies within a distance ε of an interface. This creates a line segment of width 2ε about each interface, such that if $\boldsymbol{x}$ is in one of these segments, then an interface intersects the pathline within V. Over a very large length of this line, spanning m chunks of material 1 and m chunks of material 2 (with $m \to \infty$), we have

$$\begin{aligned} (2m)(2\varepsilon) &= 4m\varepsilon \\ &= \begin{pmatrix} \text{the length of the line segments such that if } \boldsymbol{x} \text{ lies on} \\ \text{one of these segments, then an interface intersects } V \end{pmatrix} \end{aligned} \tag{47a}$$

and

$$m(\Lambda_1 + \Lambda_2) = (\text{total length of the line}), \tag{47b}$$

where Λ_i is the mean chord length in material i. The ratio of these equations is P^*. That is,

$$P^* = \frac{4\varepsilon}{\Lambda_1 + \Lambda_2}. \tag{48}$$

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. (48) into Eq. (46), we obtain

$$\left\langle f_i(\mathbf{\Omega}) \right\rangle = [\Psi_j(\mathbf{\Omega}) - \Psi_i(\mathbf{\Omega})] \lim_{\epsilon \to 0} \left[\frac{1}{4\varepsilon} \left(\frac{4\varepsilon}{\Lambda_1 + \Lambda_2} \right) \right] = \frac{\Psi_j(\mathbf{\Omega}) - \Psi_i(\mathbf{\Omega})}{\Lambda_1 + \Lambda_2}. \tag{49}$$

For binary homogeneous statistics, the following identity holds:

$$p_i = \frac{\Lambda_i}{\Lambda_1 + \Lambda_2}, \quad i \in \{1, 2\}; \tag{50}$$

it follows that

$$\left\langle f_i(\mathbf{\Omega}) \right\rangle = \frac{p_j \Psi_j(\mathbf{\Omega})}{\Lambda_j} - \frac{p_i \Psi_i(\mathbf{\Omega})}{\Lambda_i}. \tag{51}$$

Equating $\Psi_i = \psi_i$, this result is the classic LP expression for the coupling term in Markovian homogeneous statistics. The LP expression is then written as

$$\begin{aligned} &\frac{1}{v} \frac{\partial (p_i \psi_i)}{\partial t} + \mathbf{\Omega} \cdot \nabla (p_i \psi_i) + \Sigma_{ti} (p_i \psi_i) = \\ &\qquad = \frac{\Sigma_{si}}{4\pi} \int_{4\pi} p_i \psi_i(\boldsymbol{x}, \mathbf{\Omega}', t) d\Omega' + p_i Q_i + \frac{p_j \psi_j}{\Lambda_j} - \frac{p_i \psi_i}{\Lambda_i}, \end{aligned} \tag{52}$$

and the general case (general scattering, energy dependent) is straightforwardly given by

$$\begin{aligned} &\frac{1}{v} \frac{\partial (p_i \psi_i)}{\partial t} + \mathbf{\Omega} \cdot \nabla (p_i \psi_i) + \Sigma_{ti}(E) (p_i \psi_i) = \\ &\quad = \int_0^\infty \int_{4\pi} \Sigma_{si}(E \to E', \mathbf{\Omega} \cdot \mathbf{\Omega}') p_i \psi_i(\boldsymbol{x}, E', \mathbf{\Omega}', t) d\Omega' dE' + p_i Q_i + \frac{p_j \psi_j}{\Lambda_j} - \frac{p_i \psi_i}{\Lambda_i}, \end{aligned} \tag{53}$$

In order to extend these considerations to nonstatic physical realizations of the mixing, we define

$$\chi_i(\boldsymbol{x}, t) = \begin{cases} 1, & \text{if } \boldsymbol{x} \text{ is in material } i \text{ at time } t \\ 0, & \text{if } \boldsymbol{x} \text{ is in material } j \neq i \text{ at time } t \end{cases}. \tag{54}$$

Applying the same procedure as before, a new term will appear, given by (h_i) in

$$\frac{1}{v}\left(\chi_i\frac{\partial\psi}{\partial t}\right) = \frac{1}{v}\frac{\partial(\chi_i\psi)}{\partial t} \quad - \quad \underbrace{\frac{1}{v}\left(\psi\frac{\partial\chi_i}{\partial t}\right)}_{(h_i)}. \tag{55}$$

We define $p_i(\boldsymbol{x},t)$, the probability of finding material i at point $\boldsymbol{x}$ and time t, by

$$p_i(\boldsymbol{x},t) = \big\langle \chi_i(\boldsymbol{x},t)\big\rangle, \tag{56}$$

and the ensemble-averaged angular flux over all physical realizations such that $\boldsymbol{x}$ is in material i at time t by

$$\psi_i(\boldsymbol{x},E,\boldsymbol{\Omega},t) = \frac{\big\langle \chi_i(\boldsymbol{x},t)\psi(\boldsymbol{x},E,\boldsymbol{\Omega},t)\big\rangle}{\big\langle \chi_i(\boldsymbol{x},t)\big\rangle}. \tag{57}$$

Treating $\big\langle h_i\big\rangle$ in analogy with the way we treated $\big\langle f_i\big\rangle$, we find

$$\begin{aligned}\frac{1}{v}\frac{\partial(p_i\psi_i)}{\partial t} + \boldsymbol{\Omega}\cdot\nabla(p_i\psi_i) + \Sigma_{ti}(p_i\psi_i) = \\ \int_0^\infty\int_{4\pi}\Sigma_{si}(E\to E',\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')p_i\psi_i(\boldsymbol{x},E',\boldsymbol{\Omega}',t)d\Omega' dE' + \\ + p_iQ_i + \left(\frac{p_j\Psi_j}{\Lambda_j} - \frac{p_i\Psi_i}{\Lambda_i}\right) + \left(\frac{p_j\hat{\Psi}_j}{\hat{\lambda}_j} - \frac{p_i\hat{\Psi}_i}{\hat{\lambda}_i}\right),\end{aligned} \tag{58}$$

where

$$\frac{p_i(\boldsymbol{x},t)}{\hat{\lambda}_i(\boldsymbol{x},t)} = \frac{1}{v}\lim_{T\to 0}\left[\frac{1}{T}\big\langle N_i\big\rangle\right] \tag{59}$$

and

$$\hat{\Psi}_i = \big\langle\psi\big\rangle^{\ddagger}_{i\to j}. \tag{60}$$

In Eq. (59), T is a time interval and N_i is the number of transitions from material i to material $j\neq i$ in T at space point $\boldsymbol{x}$. In Eq. (60), the operator $\big\langle\,\cdot\,\big\rangle^{\ddagger}_{i\to j}$ is a restricted average, defined to be an ensemble average over realizations that undergo a transition from material i to material j at a given space point $\boldsymbol{x}$ at a time t.

Again, a simple closure is obtained by setting $\Psi_i = \hat{\Psi}_i = \psi_i$. Also, we can define a composite coupling coefficient $\tilde{\lambda}_i$ according to

$$\frac{1}{\tilde{\lambda}_i} = \frac{1}{\Lambda_i} + \frac{1}{\hat{\lambda}_i}, \tag{61}$$

and applying these arguments in Eq. (58), it becomes identical to Eq. (53) (with the terms Λ_i replaced by $\tilde{\lambda}_i$).

References

[1] DUMAS, L. AND GOLSE, F. "Homogenization of Transport Equations", *SIAM J. Appl. Math.* **60** (2000), 1447.

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

[3] LARSEN, E. W., VASQUES, R., AND VILHENA, M. T. "Particle Transport in the 1-D Diffusive Atomic Mix Limit", in *Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications.* Avignon, France (2005), in CD-ROM.

[4] ADAMS, M. L., LARSEN, E. W., AND POMRANING, G. C. "Benchmark Results for Particle Transport in a Binary Markov Statistical Medium", *J. Quant. Spectrosc. Radiat. Transfer* **42** (1989), 253.

[5] VASQUES, R., VILHENA, M. T., THOMPSON, M., AND LARSEN, E. W. "State of Art of Particle Transport Theory in Stochastic Media", in *Proc. XXV Iberian Latin American Congress on Computational Methods in Engineering*, Recife (2004), on CD-ROM.