Annals of Nuclear Energy 70 (2014) 292–300

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Non-classical particle transport with angular-dependent path-length distributions. I: Theory

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ARTICLE INFO

Article history:
Received 5 October 2013
Accepted 30 December 2013
Available online 31 January 2014

Keywords:
Particle transport
Random media
Correlated scattering centers

ABSTRACT

This paper extends a recently introduced theory describing particle transport for random statistically homogeneous systems in which the distribution function $p(s)$ for chord lengths between scattering centers is non-exponential. Here, we relax the previous assumption that $p(s)$ does not depend on the direction of flight $\mathbf{\Omega}$; this leads to a new generalized linear Boltzmann equation that includes angular-dependent cross sections, and to a new generalized diffusion equation that accounts for anisotropic behavior resulting from the statistics of the system.

1. Introduction

The classical theory of linear particle transport defines as $dp = \Sigma_t(\boldsymbol{x}, E)ds$ the incremental probability dp that a particle at point $\boldsymbol{x}$ with energy E will experience an interaction while traveling an incremental distance ds in the background material. Here, the total cross section Σ_t is independent of the direction of flight $\mathbf{\Omega}$, and the path-length s is defined as

$$s = \text{the path-length traveled by the particle since its previous interaction(birth or scattering)}. \tag{1.1}$$

This typically leads to the particle flux decreasing as an exponential function of the path-length (Beer–Lambert law).

However, in an inhomogeneous random medium, particles will travel through different materials with randomly located interfaces. In atmospheric clouds, experimental studies have found evidence of a non-exponential attenuation law (Davis et al., 1996; Marshak et al., 1997; Pfeilsticker, 1999). It has been suggested (Kostinski, 2001) that the locations of the scattering centers (in this case water droplets) are spatially correlated in ways that measurably affect radiative transfer within the cloud (Kostinski and Shaw, 2001; Buldyrev et al., 2001; Shaw et al., 2002; Davis, 2008; Borovoi, 2002; Kostinski, 2002; Davis and Marshak, 2004; Scholl et al., 2006).

An approach to this type of non-classical transport problem was recently introduced (Larsen, 2007), with the assumption that the positions of the scattering centers are correlated but independent of direction $\mathbf{\Omega}$; that is, Σ_t is independent of $\mathbf{\Omega}$ but not $s : \Sigma_t = \Sigma_t(\boldsymbol{x}, E, s)$. A full derivation of this generalized linear Boltzmann equation (GLBE) and its asymptotic diffusion limit can be found in Larsen and Vasques (2011), along with numerical results for an application in 2-D pebble bed reactor (PBR) cores. Existence and uniqueness of solutions, as well as their convergence to the diffusion equation, are rigorously discussed in Frank and Goudon (2010). Furthermore, a similar kinetic equation with path-length as an independent variable has been derived for the periodic Lorentz gas (Golse, 2012).

For specific random systems in which the locations of the scattering centers are correlated and dependent on the direction $\mathbf{\Omega}$, anisotropic particle transport arises (Vasques, 2009; Vasques and Larsen, 2009). This anisotropy is a direct result of the geometry of the random system – for instance, the packing of pebbles close to the boundaries of a pebble bed system leads to particles traveling longer distances in directions parallel to the boundary wall (Vasques, 2013). One may also expect that, due to the "gravitational" arrangement of pebbles in PBR cores, diffusion in the vertical and horizontal directions might differ. This behavior can only be captured if we allow the path-lengths of the particles to depend upon $\mathbf{\Omega}$; that is, $\Sigma_t = \Sigma_t(\boldsymbol{x}, \mathbf{\Omega}, E, s)$. (Implications of angular-dependent cross-sections in anisotropic media have been previously considered in Williams (1978), in connection with charged particle transport in lattice-like structures.)

The goal of this paper is to extend the GLBE formulation in Larsen and Vasques (2011) to include this angular dependence. For simplicity, we do not consider the most general problem here; similarly to Larsen and Vasques (2011), our analysis is based on five primary assumptions:

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0306-4549/$ - see front matter
http://dx.doi.org/10.1016/j.anucene.2013.12.021

i. The physical system is infinite and statistically homogeneous.
ii. Particle transport is monoenergetic. (However, the inclusion of energy- or frequency-dependence is straightforward.)
iii. Particle transport is driven by a known interior isotropic source $Q(\boldsymbol{x})$ satisfying $Q \to 0$ as $|\boldsymbol{x}| \to \infty$ (and the particle flux $\to 0$ as $|\boldsymbol{x}| \to \infty$).
iv. The ensemble averaged total cross section $\Sigma_t(\boldsymbol{\Omega}, s)$, defined as

$$\Sigma_t(\boldsymbol{\Omega}, s)ds = \text{the probability(ensemble-averaged over all physical realizations)that a particle, scattered or born at any point } \boldsymbol{x} \text{ and traveling in the direction } \boldsymbol{\Omega}, \text{ will experience a collision between } \boldsymbol{x} + s\boldsymbol{\Omega} \text{ and } \boldsymbol{x} + (s + ds)\boldsymbol{\Omega},$$

is known. (In the next part of this 2-part paper we discuss how $\Sigma_t(\boldsymbol{\Omega}, s)$ might be numerically derived from hypothesized correlations between the scattering centers.)
v. The distribution function $P(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$ for scattering from $\boldsymbol{\Omega}'$ to $\boldsymbol{\Omega}$ is independent of s. (The correlation in the scattering center positions affects the probability of collision, but not the scattering properties when scattering events occur.)

For problems in general random media, $\Sigma_t(\boldsymbol{\Omega}, s)$ depends also on $\boldsymbol{x}$. In this paper the statistics are assumed to be homogeneous, in which case the dependence on $\boldsymbol{x}$ is dropped. (In the derivation of the GLBE in Larsen and Vasques (2011), the statistics was assumed to be independent of $\boldsymbol{x}$ and $\boldsymbol{\Omega}$.)

A summary of the remainder of the paper follows. In Section 2 we present definitions and formally derive the new GLBE. In Section 3 we derive (i) the conditional distribution function $q(\boldsymbol{\Omega}, s)$ for the distance s to collision in a given direction $\boldsymbol{\Omega}$ in terms of the total cross section $\Sigma_t(\boldsymbol{\Omega}, s)$; and (ii) the equilibrium path-length spectrum in a given direction. In Section 4 we reformulate the new GLBE in terms of integral equations in which s is absent. In Section 5 we derive the asymptotic diffusion limit of the new GLBE, presenting 3 physically relevant special cases; and in Section 6 we show that if $\Sigma_t(\boldsymbol{\Omega}, s)$ is independent of both $(\boldsymbol{\Omega}, s)$, the theory introduced here reduces to the classical theory. We conclude with a discussion in Section 7.

2. Derivation of the new GLBE

Using the notation $\boldsymbol{x} = (x, y, z) =$ position and $\boldsymbol{\Omega} = (\Omega_x, \Omega_y, \Omega_z) =$ direction of flight (with $|\boldsymbol{\Omega}| = 1$), and using Eq. (1.1) for s, we define:

$$n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds = \text{the number of particles in } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s), \tag{2.1a}$$

$$v = \frac{ds}{dt} = \text{the particle speed}, \tag{2.1b}$$

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = vn(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \text{the angular flux}, \tag{2.1c}$$

$$\Sigma_t(\boldsymbol{\Omega}, s)ds = \text{the probability that a particle that has traveled a distance s in the direction } \boldsymbol{\Omega} \text{ since its previous interaction (birth or scattering) will experience its next interaction while traveling a further distance } ds, \tag{2.1d}$$

$$c = \text{the probability that when a particle experiences a collision, it will scatter (notice that } c \text{ is independent of } s \text{ and } \boldsymbol{\Omega}), \tag{2.1e}$$

$$P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})d\Omega = \text{the probability that when a particle with direction of flight } \boldsymbol{\Omega}' \text{ scatters, its outgoing direction of flight will lie in } d\Omega \text{ about } \boldsymbol{\Omega} \ (P \text{ is independent of } s), \tag{2.1f}$$

$$Q(\boldsymbol{x})dV = \text{the rate at which source particles are isotropically emitted by an internal source } Q(\boldsymbol{x}) \text{ in } dV \text{ about } \boldsymbol{x}. \tag{2.1g}$$

Classic manipulations directly lead to:

$$\begin{aligned}\frac{\partial}{\partial s}\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds &= \frac{1}{v}\frac{\partial}{\partial t}vn(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds \\ &= \frac{\partial}{\partial t}n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds \\ &= \text{the rate of change of the number of particles in } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s),\end{aligned} \tag{2.2a}$$

$$|\boldsymbol{\Omega} \cdot \mathbf{n}|\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dS\, d\Omega\, ds = \text{the rate at which particles in } d\Omega\, ds \text{ about } (\boldsymbol{\Omega}, s) \text{ flow through an incremental surface area } dS \text{ with unit normal vector } \mathbf{n}, \tag{2.2b}$$

$$\boldsymbol{\Omega} \cdot \nabla\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds = \text{the net rate at which particles in } d\Omega\, ds \text{ about } (\boldsymbol{\Omega}, s) \text{ flow (leak) out of } dV \text{ about } \boldsymbol{x}, \tag{2.2c}$$

$$\begin{aligned}\Sigma_t(\boldsymbol{\Omega}, s)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds &= \Sigma_t(\boldsymbol{\Omega}, s)\frac{ds}{dt}n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds \\ &= \frac{1}{dt}[\Sigma_t(\boldsymbol{\Omega}, s)ds][n(\boldsymbol{x}, \boldsymbol{\Omega}, s)dV\, d\Omega\, ds] \\ &= \text{the rate at which particles in } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s) \text{ experience collisions}.\end{aligned} \tag{2.2d}$$

The treatment of the inscattering and source terms requires extra care. From Eq. (2.2d),

$$\left[\int_0^\infty \Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\right]dV\, d\Omega' = \text{the rate at which particles in } dV\, d\Omega' \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}') \text{ experience collisions}.$$

Multiplying this expression by $cP(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')d\Omega$, we obtain:

$$cP(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')\left[\int_0^\infty \Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\right]dV\, d\Omega'\, d\Omega = \text{the rate at which particles in } dV\, d\Omega' \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}') \text{ scatter into } dV\, d\Omega \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}).$$

Integrating this expression over $\boldsymbol{\Omega}' \in 4\pi$, we get:

$$\left[c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\, d\Omega'\right]dV\, d\Omega = \text{the rate at which particles scatter into } dV\, d\Omega \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}).$$

Finally, when particles emerge from a scattering event their value of s is "reset" to $s = 0$. Therefore, the path-length spectrum of particles that emerge from scattering events is the delta function $\delta(s)$. Multiplying the previous expression by $\delta(s)ds$, we obtain:

$$\left[\delta(s)c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\, d\Omega'\right]dV\, d\Omega\, ds = \text{the rate at which particles scatter into } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s). \tag{2.2e}$$

Also,

$$\delta(s)\frac{Q(\boldsymbol{x})}{4\pi}dV\, d\Omega\, ds = \text{the rate at which source particles are emitted into } dV\, d\Omega\, ds \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}, s). \tag{2.2f}$$

We now use the familiar conservation equation (in each of the following terms, the phrase "of particles in $dV\,d\Omega\,ds$ about $(\boldsymbol{x}, \boldsymbol{\Omega}, s)$" is omitted):

$$\begin{aligned}\text{Rate of change} &= \text{Rate of gain} - \text{Rate of loss}\\ &= (\text{Inscatter rate} + \text{Source rate})\\ &\quad - (\text{Net leakage rate} + \text{Collision rate}).\end{aligned} \tag{2.3}$$

Introducing Eqs. (2.2) into this expression and dividing by $dV\,d\Omega\,ds$, we obtain the new GLBE for $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)$:

$$\begin{aligned}&\frac{\partial\psi}{\partial s}(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \Sigma_t(\boldsymbol{\Omega}, s)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)\\ &\quad = \delta(s)\; c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\Omega'\\ &\quad + \delta(s)\frac{Q(\boldsymbol{x})}{4\pi}.\end{aligned}$$

Eq. (2.4) can be written in a mathematically equivalent way in which the delta function is not present: for $s > 0$

$$\frac{\partial\psi}{\partial s}(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \Sigma_t(\boldsymbol{\Omega}, s)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = 0; \tag{2.5a}$$

then, operating on Eq. (2.4) by $\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon}(\cdot)ds$ and using $\psi = 0$ for $s < 0$, we obtain

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = c\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\Sigma_t(\boldsymbol{\Omega}', s')\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'\,d\Omega' + \frac{Q(\boldsymbol{x})}{4\pi}. \tag{2.5b}$$

Eqs. (2.5) are mathematically equivalent to Eq. (2.4).

To establish the relationship between the present work and the classic number density and angular flux, we integrate Eq. (2.1a) over s and obtain:

$$\left[\int_0^\infty n(\boldsymbol{x}, \boldsymbol{\Omega}, s)ds\right]dV\,d\Omega = \text{the total number of particles in } dV\,d\Omega \text{ about } (\boldsymbol{x}, \boldsymbol{\Omega}). \tag{2.6}$$

Therefore,

$$n_c(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty n(\boldsymbol{x}, \boldsymbol{\Omega}, s)ds = \text{classic number density}, \tag{2.7}$$

and

$$\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}) = v n_c(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)ds = \text{classic angular flux}. \tag{2.8}$$

3. The angular-dependent path-length and equilibrium path-length distributions

Without loss of generality, let us consider a single particle released from an interaction site at $x = 0$ in the direction $\boldsymbol{\Omega} = \boldsymbol{i}$ = direction of the positive x-axis. Eq. (2.5a) for this particle becomes:

$$\frac{\partial\psi}{\partial s}(x, \boldsymbol{\Omega} = \boldsymbol{i}, s) + \frac{\partial\psi}{\partial x}(x, \boldsymbol{\Omega} = \boldsymbol{i}, s) + \Sigma_t(\boldsymbol{\Omega} = \boldsymbol{i}, s)\psi(x, \boldsymbol{\Omega} = \boldsymbol{i}, s) = 0. \tag{3.1}$$

For this particle, we have $x(s) = s$ and $\psi(x(s), \boldsymbol{i}, s) \equiv F(\boldsymbol{i}, s)$. Therefore,

$$\frac{dF}{ds}(\boldsymbol{i}, s) = \frac{\partial\psi}{\partial x}(x(s), \boldsymbol{i}, s)\left(\frac{dx}{ds}\right) + \frac{\partial\psi}{\partial s}(x(s), \boldsymbol{i}, s) = \frac{\partial\psi}{\partial x} + \frac{\partial\psi}{\partial s} \tag{3.2}$$

Eq. (3.1) then simplifies to:

$$\frac{dF}{ds}(\boldsymbol{i}, s) + \Sigma_t(\boldsymbol{i}, s)F(\boldsymbol{i}, s) = 0. \tag{3.3a}$$

We apply the initial condition

$$F(\boldsymbol{i}, 0) = 1, \tag{3.3b}$$

since we are considering a single particle. The solution of Eqs. (3.3) is:

$$\begin{aligned}F(\boldsymbol{\Omega} = \boldsymbol{i}, s) = e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}=\boldsymbol{i}, s')ds'} &= \text{the probability that the particle will travel the distance } s \text{ in the given direction } \boldsymbol{\Omega}\\ &= \boldsymbol{i} \text{ without interacting.}\end{aligned} \tag{3.4}$$

We can generalize this equation for all directions, giving

$$F(\boldsymbol{\Omega}, s) = e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'} = \text{the probability that the particle will travel the distance } s \text{ in a given direction } \boldsymbol{\Omega} \text{ without interacting.} \tag{3.5}$$

The probability of a collision between s and $s + ds$ in a given direction $\boldsymbol{\Omega}$ is:

$$\Sigma_t(\boldsymbol{\Omega}, s)F(\boldsymbol{\Omega}, s)ds = q(\boldsymbol{\Omega}, s)ds, \tag{3.6}$$

and therefore:

$$\begin{aligned}q(\boldsymbol{\Omega}, s) &= \Sigma_t(\boldsymbol{\Omega}, s)e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}\\ &= \text{conditional distribution function for the distance} - \text{to} - \text{collision in a given direction } \boldsymbol{\Omega}.\end{aligned} \tag{3.7}$$

Let us define

$$\xi(\boldsymbol{\Omega})d\Omega = \text{probability that a particle is traveling in } d\Omega \text{ about } \boldsymbol{\Omega}; \tag{3.8}$$

and

$$p(\boldsymbol{\Omega}, s)d\Omega\,ds = \text{probability that a particle traveling in } d\Omega \text{ about } \boldsymbol{\Omega} \text{ will experience a collision between } s \text{ and } s + ds. \tag{3.9}$$

Then

$$\begin{aligned}p(\boldsymbol{\Omega}, s)d\Omega\,ds &= (\text{prob. that a particle is traveling in } d\Omega \text{ about } \boldsymbol{\Omega})\\ &\quad \times (\text{prob. of a collision between } s \text{ and } s + ds \text{ in a given direction } \boldsymbol{\Omega})\\ &= (\xi(\boldsymbol{\Omega})d\Omega)(q(\boldsymbol{\Omega}, s)ds);\end{aligned} \tag{3.10}$$

that is, $p(\boldsymbol{\Omega}, s)$ is a joint distribution function.

Eq. (3.7) expresses $q(\boldsymbol{\Omega}, s)$ in terms of $\Sigma_t(\boldsymbol{\Omega}, s)$. To express $\Sigma_t(\boldsymbol{\Omega}, s)$ in terms of $q(\boldsymbol{\Omega}, s)$, we operate on Eq. (3.7) by $\int_0^s(\cdot)ds'$ and get:

$$\int_0^s q(\boldsymbol{\Omega}, s')ds' = 1 - e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}, \tag{3.11a}$$

or

$$e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'} = 1 - \int_0^s q(\boldsymbol{\Omega}, s')ds'. \tag{3.11b}$$

Hence,

$$\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds' = -\ln\left(1 - \int_0^s q(\boldsymbol{\Omega}, s')ds'\right). \tag{3.11c}$$

Differentiating with respect to s, we obtain:

$$\Sigma_t(\boldsymbol{\Omega}, s) = \frac{q(\boldsymbol{\Omega}, s)}{1 - \int_0^s q(\boldsymbol{\Omega}, s')ds'}. \tag{3.12}$$

Eqs. (3.7) and (3.12) show that $q(\boldsymbol{\Omega}, s)$ is exponential if and only if $\Sigma_t(\boldsymbol{\Omega}, s)$ is independent of s.

Moreover, for the case of an infinite medium with an "equilibrium" intensity having no space dependence (but dependent on direction), Eq. (2.5a) for $s > 0$ reduces to:

$$\frac{\partial \psi}{\partial s}(\boldsymbol{\Omega}, s) + \Sigma_t(\boldsymbol{\Omega}, s)\psi(\boldsymbol{\Omega}, s) = 0, \tag{3.13}$$

which has the solution

$$\psi(\boldsymbol{\Omega}, s) = \psi(\boldsymbol{\Omega}, 0)e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}. \tag{3.14}$$

Normalizing this solution to have integral = unity, we obtain:

$$\begin{aligned}\chi(\boldsymbol{\Omega}, s) &= \frac{e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}}{\int_0^\infty e^{-\int_0^{s'} \Sigma_t(\boldsymbol{\Omega}, s'')ds''} ds'} \\ &= \text{equilibrium spectrum of} \\ &\quad \text{path} - \text{length } s \text{ in a given direction } \boldsymbol{\Omega}.\end{aligned} \tag{3.15}$$

From Eq. (3.7), the mean distance-to-collision (mean free path) in a given direction $\boldsymbol{\Omega}$ is:

$$\begin{aligned}s_\Omega(\boldsymbol{\Omega}) &= \int_0^\infty s q(\boldsymbol{\Omega}, s)ds = \int_0^\infty s\left[\Sigma_t(\boldsymbol{\Omega}, s)e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}\right]ds \\ &= s\left[-e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}\right]_0^\infty - \int_0^\infty \left[-e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}\right]ds \\ &= \int_0^\infty e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'} ds.\end{aligned} \tag{3.16}$$

Eq. (3.15) can then be written:

$$\chi(\boldsymbol{\Omega}, s) = \frac{e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}}{s_\Omega(\boldsymbol{\Omega})}, \tag{3.17}$$

and by the Law of Total Expectation (Billingsley, 1995), the mean free path $\langle s \rangle$ is given by

$$\langle s \rangle = \int_{4\pi}\int_0^\infty sp(\boldsymbol{\Omega}, s)ds\, d\Omega = \int_{4\pi} \xi(\boldsymbol{\Omega})s_\Omega(\boldsymbol{\Omega})d\Omega. \tag{3.18}$$

Note: from now on we assume that $s_\Omega(\boldsymbol{\Omega})$ is an *even* function of the direction of flight $\boldsymbol{\Omega}$. This makes sense since, from the physical point of view, the mean free path of a particle traveling in the direction $\boldsymbol{\Omega}$ *must* be equal to the mean free path of a particle traveling in the direction $-\boldsymbol{\Omega}$.

4. Integral equation formulations of the new GLBE

Using the work in Larsen and Vasques (2011) as a guide, let us define:

$$f(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \Sigma_t(\boldsymbol{\Omega}, s)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s)ds = \text{collision rate density}, \tag{4.1}$$

and

$$\begin{aligned}g(\boldsymbol{x}, \boldsymbol{\Omega}) &= c\int_{4\pi} P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})f(\boldsymbol{x}, \boldsymbol{\Omega}')d\Omega' \\ &= \text{inscattering rate density}.\end{aligned} \tag{4.2}$$

The definition (4.1) allows us to rewrite Eqs. (2.5) as:

$$\frac{\partial \psi}{\partial s}(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega} \cdot \nabla\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \Sigma_t(\boldsymbol{\Omega}, s)\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = 0, \tag{4.3a}$$

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = c\int_{4\pi} P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})f(\boldsymbol{x}, \boldsymbol{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x})}{4\pi}. \tag{4.3b}$$

Solving Eq. (4.3a) and using Eq. (4.3b), we obtain for $s > 0$

$$\begin{aligned}\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) &= \psi(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}, 0)e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'} \\ &= \left[c\int_{4\pi} P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})f(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x} - s\boldsymbol{\Omega})}{4\pi}\right]e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'}.\end{aligned} \tag{4.4}$$

Operating on this equation by $\int_0^\infty \Sigma_t(\boldsymbol{\Omega}, s)(\cdot)ds$ and using Eqs. (4.1) and (3.7), we get:

$$f(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \left[c\int_{4\pi} P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})f(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x} - s\boldsymbol{\Omega})}{4\pi}\right]q(\boldsymbol{\Omega}, s)ds. \tag{4.5a}$$

Also, operating on Eq. (4.4) by $\int_0^\infty(\cdot)ds$ and using Eq. (2.8), we obtain:

$$\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \left[c\int_{4\pi} P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})f(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x} - s\boldsymbol{\Omega})}{4\pi}\right]e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'} ds. \tag{4.5b}$$

Thus, if the integral Eq. (4.5a) for $f(\boldsymbol{x}, \boldsymbol{\Omega})$ is solved, Eq. (4.5b) yields the classic angular flux.

Using definition (4.2), we can rewrite Eq. (4.5a) as:

$$f(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \left[g(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}) + \frac{Q(\boldsymbol{x} - s\boldsymbol{\Omega})}{4\pi}\right]q(\boldsymbol{\Omega}, s)ds, \tag{4.6}$$

and operating on this result by $c\int_{4\pi} P(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')(\cdot)d\Omega'$ we obtain:

$$\begin{aligned}g(\boldsymbol{x}, \boldsymbol{\Omega}) = c\int_{4\pi} P(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')\int_0^\infty &[g(\boldsymbol{x} - s\boldsymbol{\Omega}', \boldsymbol{\Omega}') \\ &+ \frac{Q(\boldsymbol{x} - s\boldsymbol{\Omega}')}{4\pi}\Big]q(\boldsymbol{\Omega}', s)ds\, d\Omega'.\end{aligned} \tag{4.7}$$

Changing the spatial variables from the 3-D spherical $(\boldsymbol{\Omega}', s)$ to the 3-D Cartesian $\boldsymbol{x}'$ defined by

$$\boldsymbol{x}' = \boldsymbol{x} - s\boldsymbol{\Omega}', \tag{4.8}$$

we obtain

$$s = |\boldsymbol{x} - \boldsymbol{x}'|, \tag{4.9a}$$

$$\boldsymbol{\Omega}' = \frac{\boldsymbol{x} - \boldsymbol{x}'}{|\boldsymbol{x} - \boldsymbol{x}'|}, \tag{4.9b}$$

$$s^2\, ds\, d\Omega = dV'. \tag{4.9c}$$

Now, we can rewrite Eq. (4.7) as:

$$g(\boldsymbol{x}, \boldsymbol{\Omega}) = c\iiint P\left(\frac{\boldsymbol{x} - \boldsymbol{x}'}{|\boldsymbol{x} - \boldsymbol{x}'|} \cdot \boldsymbol{\Omega}\right)\left[g\left(\boldsymbol{x}', \frac{\boldsymbol{x} - \boldsymbol{x}'}{|\boldsymbol{x} - \boldsymbol{x}'|}\right) + \frac{Q(\boldsymbol{x}')}{4\pi}\right]\frac{\hat{q}(|\boldsymbol{x} - \boldsymbol{x}'|)}{|\boldsymbol{x} - \boldsymbol{x}'|^2}dV', \tag{4.10a}$$

where $\hat{q}(|\boldsymbol{x} - \boldsymbol{x}'|)dV'$ is the conditional probability that, given the direction defined by $\boldsymbol{x} - \boldsymbol{x}'$, a particle moving from a point $\boldsymbol{x}$ to a point lying in dV' about $\boldsymbol{x}'$ will experience a collision. Definition (4.2) allows us to rewrite Eq. (4.5b) as well:

$$\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}) = \int_0^\infty \left[g(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}) + \frac{Q(\boldsymbol{x} - s\boldsymbol{\Omega})}{4\pi}\right]e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega}, s')ds'} ds. \tag{4.10b}$$

Here, solving the integral Eq. (4.10a) for $g(\boldsymbol{x}, \boldsymbol{\Omega})$, Eq. (4.10b) yields the classic angular flux. This specific formulation does not contain the path-length variable s as an independent variable.

Finally, for the case of isotropic scattering (in which $P(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}) = 1/4\pi$), $g(\boldsymbol{x}, \boldsymbol{\Omega})$ in Eq. (4.2) becomes isotropic:

$$g(\boldsymbol{x}) = \frac{c}{4\pi}\int_{4\pi} f(\boldsymbol{x}, \boldsymbol{\Omega}')d\Omega' \equiv \frac{c}{4\pi}\widehat{F}(\boldsymbol{x}), \tag{4.11a}$$

where

$$\widehat{F}(\boldsymbol{x}) = \int_{4\pi} f(\boldsymbol{x}, \boldsymbol{\Omega}')d\Omega' = \text{scalar collision rate density}. \tag{4.11b}$$

Eq. (4.10a) is then reduced to

$$\widehat{F}(\boldsymbol{x}) = \iiint [c\widehat{F}(\boldsymbol{x}') + Q(\boldsymbol{x}')]\frac{\hat{q}(|\boldsymbol{x} - \boldsymbol{x}'|)}{4\pi|\boldsymbol{x} - \boldsymbol{x}'|^2}dV'; \tag{4.12a}$$

and using Eq. (4.11a), we write Eq. (4.10b) as:

$$\psi_c(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{1}{4\pi}\int_0^\infty [c\widehat{F}(\boldsymbol{x}-s\boldsymbol{\Omega}) + Q(\boldsymbol{x}-s\boldsymbol{\Omega})]e^{-\int_0^s \Sigma_t(\boldsymbol{\Omega},s')ds'}\,ds. \tag{4.12b}$$

Operating on this equation by $\int_{4\pi}(\cdot)d\Omega$ and using Eqs. (48) and (49), we obtain:

$$\phi_c(\boldsymbol{x}) = \iiint [c\widehat{F}(\boldsymbol{x}') + Q(\boldsymbol{x}')]\frac{e^{-\int_0^{|\boldsymbol{x}-\boldsymbol{x}'|}\Sigma_t\left(\frac{\boldsymbol{x}-\boldsymbol{x}'}{|\boldsymbol{x}-\boldsymbol{x}'|},s'\right)ds'}}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|^2}dV'. \tag{4.12c}$$

If we solve the integral Eq. (4.12a) for $\widehat{F}(\boldsymbol{x})$, the classic angular flux is given by Eq. (4.12b) and the classic scalar flux is given by Eq. (4.12c).

5. Asymptotic diffusion limit of the new GLBE

To begin this discussion, we must first consider the Legendre polynomial expansion of the distribution function $P(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = P(\mu_0)$ defined by Eq. (2.1f) (Lewis and Miller, 1993):

$$P(\mu_0) = \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}a_n P_n(\mu_0), \tag{5.1}$$

where $a_0 = 1$ and $a_1 = \bar{\mu}_0$ = mean scattering cosine. We define $P^*(\mu_0)$ by:

$$P^*(\mu_0) = cP(\mu_0) + \frac{1-c}{4\pi}, \tag{5.2}$$

which has the Legendre polynomial expansion:

$$P^*(\mu_0) = \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}a_n^* P_n(\mu_0), \tag{5.3a}$$

$$a_n^* = \begin{cases} 1, & n = 0, \\ ca_n, & n \geqslant 1. \end{cases} \tag{5.3b}$$

Using the work in Larsen et al. (1996) as a guide, we scale $\Sigma_t = O(\varepsilon^{-1}), 1-c = O(\varepsilon^2)$, $Q = O(\varepsilon), P^*(\mu_0)$ is independent of ε, and $\partial\psi/\partial s = O(\varepsilon^{-1})$, with $\varepsilon \ll 1$. Eqs. (2.4) and (5.2) yield, in this scaling,

$$\begin{aligned}\frac{1}{\varepsilon}\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x},\boldsymbol{\Omega},s) + \frac{\Sigma_t(\boldsymbol{\Omega},s)}{\varepsilon}\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \\ \delta(s)\int_{4\pi}\int_0^\infty\left[P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') - \varepsilon^2\frac{1-c}{4\pi}\right]\frac{\Sigma_t(\boldsymbol{\Omega}',s')}{\varepsilon}\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' \\ + \varepsilon\delta(s)\frac{Q(\boldsymbol{x})}{4\pi}.\end{aligned} \tag{5.4}$$

Let us define $\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)$ by:

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s) \equiv \Psi(\boldsymbol{x},\boldsymbol{\Omega},s)\frac{e^{-\int_0^s\Sigma_t(\boldsymbol{\Omega},s')ds'}}{\langle s\rangle}. \tag{5.5}$$

Then, using Eqs. (3.7) and (5.4) for $\psi(\boldsymbol{x},\boldsymbol{\Omega},s)$ becomes the following equation for $\Psi(\boldsymbol{x},\boldsymbol{\Omega},s)$:

$$\begin{aligned}\frac{\partial\Psi}{\partial s}&(\boldsymbol{x},\boldsymbol{\Omega},s) + \varepsilon\boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) \\ &= \delta(s)\int_{4\pi}\int_0^\infty\left[P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') - \varepsilon^2\frac{1-c}{4\pi}\right]q(\boldsymbol{\Omega}',s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' \\ &+ \varepsilon^2\delta(s)\langle s\rangle\frac{Q(\boldsymbol{x})}{4\pi}.\end{aligned} \tag{5.6}$$

The scaling in this equation implies the following:

- The $O(1)$ terms describe particle scattering. The transport process is dominated by scattering; the length scale for the problem is chosen so that a unit of length is comparable to a typical mean free path, and the system is many mean free paths thick.
- The leakage $(\boldsymbol{\Omega}\cdot\nabla\Psi)$ term is $O(\varepsilon)$. (The angular flux ψ varies a small amount over the distance of one mean free path.)
- The absorption term $1-c = \Sigma_a/\Sigma_t$ and the source term Q are $O(\varepsilon^2)$, balanced in such a way that the infinite medium solution $\psi = Q/4\pi\Sigma_a$ is $O(1)$. (The infinite medium solution holds when the source and the cross sections are constant.)
- In the scaling defined by Eqs. (5.3) only the $n = 0$ constant a_0 is "stretched" asymptotically; the higher-order $(n \geqslant 1)$ terms are not stretched. When this scaling is applied to a standard linear Boltzmann equation one obtains the same diffusion equation that is obtained from the standard P_1 or spherical harmonics approximation.

Eq. (5.6) is mathematically equivalent to:

$$\frac{\partial\Psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s) + \varepsilon\boldsymbol{\Omega}\cdot\nabla\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) = 0, \quad s > 0, \tag{5.7a}$$

$$\begin{aligned}\Psi(\boldsymbol{x},\boldsymbol{\Omega},0) = \int_{4\pi}\left[P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') - \varepsilon^2\frac{1-c}{4\pi}\right]\int_0^\infty q(\boldsymbol{\Omega}',s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' \\ + \varepsilon^2\langle s\rangle\frac{Q(\boldsymbol{x})}{4\pi}.\end{aligned} \tag{5.7b}$$

Integrating Eq. (5.7a) over $0 < s' < s$, we obtain:

$$\begin{aligned}\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) &= \Psi(\boldsymbol{x},\boldsymbol{\Omega},0) - \varepsilon\boldsymbol{\Omega}\cdot\nabla\int_0^s\Psi(\boldsymbol{x},\boldsymbol{\Omega},s')ds' \\ &= \int_{4\pi}\left[P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') - \varepsilon^2\frac{1-c}{4\pi}\right]\int_0^\infty q(\boldsymbol{\Omega}',s')\Psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' \\ &+ \varepsilon^2\langle s\rangle\frac{Q(\boldsymbol{x})}{4\pi} - \varepsilon\boldsymbol{\Omega}\cdot\nabla\int_0^s\Psi(\boldsymbol{x},\boldsymbol{\Omega},s')ds'.\end{aligned} \tag{5.8}$$

Introducing into this equation the ansatz

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \sum_{n=0}^\infty\varepsilon^n\Psi^{(n)}(\boldsymbol{x},\boldsymbol{\Omega},s) \tag{5.9}$$

and equating the coefficients of different powers of ε, we obtain for $n \geqslant 0$:

$$\begin{aligned}\Psi^{(n)}(\boldsymbol{x},\boldsymbol{\Omega},s) &= \int_{4\pi}P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\int_0^\infty q(\boldsymbol{\Omega}',s')\Psi^{(n)}(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' \\ &- \boldsymbol{\Omega}\cdot\nabla\int_0^s\Psi^{(n-1)}(\boldsymbol{x},\boldsymbol{\Omega},s')ds' \\ &- \frac{1-c}{4\pi}\int_{4\pi}\int_0^\infty q(\boldsymbol{\Omega}',s')\Psi^{(n-2)}(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' \\ &+ \delta_{n,2}\langle s\rangle\frac{Q(\boldsymbol{x})}{4\pi}.\end{aligned} \tag{5.10}$$

We solve these equations recursively, using the Legendre polynomial expansion (5.2) of $P^*(\mu_0)$.

Eq. (5.10) with $n = 0$ is:

$$\Psi^{(0)}(\boldsymbol{x},\boldsymbol{\Omega},s) = \int_{4\pi}P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\int_0^\infty q(\boldsymbol{\Omega}',s')\Psi^{(0)}(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega'. \tag{5.11}$$

The general solution of this equation is:

$$\Psi^{(0)}(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{\Phi^{(0)}(\boldsymbol{x})}{4\pi}, \tag{5.12}$$

where $\Phi^{(0)}(\boldsymbol{x})$ is, at this point, undetermined.

Next, Eq. (5.10) with $n = 1$ is:

$$\begin{aligned}\Psi^{(1)}(\boldsymbol{x},\boldsymbol{\Omega},s) &= \int_{4\pi}P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\int_0^\infty q(\boldsymbol{\Omega}',s')\Psi^{(1)}(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' \\ &- s\boldsymbol{\Omega}\cdot\nabla\frac{\Phi^{(0)}(\boldsymbol{x})}{4\pi}.\end{aligned} \tag{5.13}$$

This equation has a particular solution of the form:

$$\Psi^{(1)}_{part}(\boldsymbol{x},\boldsymbol{\Omega},s) = [\boldsymbol{\tau}(\boldsymbol{\Omega}) - s\boldsymbol{\Omega}]\cdot\nabla\frac{\Phi^{(0)}(\boldsymbol{x})}{4\pi}, \tag{5.14}$$

where

$$\boldsymbol{\tau}(\boldsymbol{\Omega}) = \int_{4\pi} P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')\boldsymbol{\tau}(\boldsymbol{\Omega}')d\Omega' + \widehat{\boldsymbol{S}}(\boldsymbol{\Omega}), \tag{5.15a}$$

$$\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}) = -\int_{4\pi}\boldsymbol{\Omega}'P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')s_\Omega(\boldsymbol{\Omega}')d\Omega'. \tag{5.15b}$$

As a Fredholm integral equation of the second kind, Eq. (5.15a) has the Liouville-Neumann series solution (Arfken, 1985):

$$\boldsymbol{\tau}(\boldsymbol{\Omega}) = \lim_{N\to\infty}\sum_{n=0}^{N}\boldsymbol{\tau}_n(\boldsymbol{\Omega}), \tag{5.16}$$

where

$$\boldsymbol{\tau}_0(\boldsymbol{\Omega}) = \widehat{\boldsymbol{S}}(\boldsymbol{\Omega}), \tag{5.17a}$$

$$\boldsymbol{\tau}_1(\boldsymbol{\Omega}) = \int_{4\pi} P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}_1)\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}_1)d\Omega_1, \tag{5.17b}$$

$$\boldsymbol{\tau}_2(\boldsymbol{\Omega}) = \int_{4\pi}\int_{4\pi} P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}_1)P^*(\boldsymbol{\Omega}_1\cdot\boldsymbol{\Omega}_2)\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}_2)d\Omega_2\,d\Omega_1, \tag{5.17c}$$

$$\vdots$$

$$\begin{aligned}\boldsymbol{\tau}_n(\boldsymbol{\Omega}) = \int_{4\pi}\int_{4\pi}\dots\int_{4\pi} & P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}_1)P^*(\boldsymbol{\Omega}_1\cdot\boldsymbol{\Omega}_2)\dots \\ & \dots P^*(\boldsymbol{\Omega}_{n-1}\cdot\boldsymbol{\Omega}_n)\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}_n)d\Omega_n\dots d\Omega_2\,d\Omega_1.\end{aligned} \tag{5.17d}$$

Since $s_\Omega(\boldsymbol{\Omega})$ is an even function of $\boldsymbol{\Omega}$, we note that $\widehat{\boldsymbol{S}}(\boldsymbol{\Omega})$ and $\boldsymbol{\tau}(\boldsymbol{\Omega})$ are odd functions of $\boldsymbol{\Omega}$:

$$\begin{aligned}\widehat{\boldsymbol{S}}(-\boldsymbol{\Omega}) &= -\int_{4\pi}\boldsymbol{\Omega}'P^*(-\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')s_\Omega(\boldsymbol{\Omega}')d\Omega' \\ &= -\int_{4\pi} -\boldsymbol{\Omega}'P^*(-\boldsymbol{\Omega}\cdot-\boldsymbol{\Omega}')s_\Omega(-\boldsymbol{\Omega}')d\Omega' \\ &= \int_{4\pi}\boldsymbol{\Omega}'P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')s_\Omega(\boldsymbol{\Omega}')d\Omega' = -\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}),\end{aligned} \tag{5.18}$$

and $\boldsymbol{\tau}_n(-\boldsymbol{\Omega}) = -\boldsymbol{\tau}_n(\boldsymbol{\Omega})\ \forall n\geq 0$ follows with the same argument, by Eqs. (5.17). The general solution of Eq. (5.13) is given by:

$$\Psi^{(1)}(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{\Phi^{(1)}(\boldsymbol{x})}{4\pi} + [\boldsymbol{\tau}(\boldsymbol{\Omega}) - s\boldsymbol{\Omega}]\cdot\nabla\frac{\Phi^{(0)}(\boldsymbol{x})}{4\pi}, \tag{5.19}$$

where $\Phi^{(1)}(\boldsymbol{x})$ is undetermined.

Eq. (5.10) with $n = 2$ has a solvability condition, which is obtained by operating on it by $\int_{4\pi}\int_0^\infty q(\boldsymbol{\Omega},s)(\cdot)ds\,d\Omega$. Using Eqs. (5.12) and (5.19) to obtain:

$$\int_{4\pi}\int_0^\infty q(\boldsymbol{\Omega}',s')\Psi^{(0)}(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'\,d\Omega' = \Phi^{(0)}(\boldsymbol{x}), \tag{5.20a}$$

and:

$$\int_0^s \Psi^{(1)}(\boldsymbol{x},\boldsymbol{\Omega},s')ds' = s\frac{\Phi^{(1)}(\boldsymbol{x})}{4\pi} + \left(s\boldsymbol{\tau}(\boldsymbol{\Omega}) - \frac{s^2}{2}\boldsymbol{\Omega}\right)\cdot\nabla\frac{\Phi^{(0)}(\boldsymbol{x})}{4\pi}, \tag{5.20b}$$

the solvability condition becomes:

$$\begin{aligned}0 = \frac{1}{4\pi}\int_{4\pi}\int_0^\infty q(\boldsymbol{\Omega},s)\left(\frac{s^2}{2}[\boldsymbol{\Omega}\cdot\nabla]^2 - s[\boldsymbol{\tau}(\boldsymbol{\Omega})\cdot\nabla][\boldsymbol{\Omega}\cdot\nabla]\right)\Phi^{(0)}(\boldsymbol{x})ds\,d\Omega \\ -\frac{(1-c)}{4\pi}\int_{4\pi}\int_0^\infty q(\boldsymbol{\Omega},s)\Phi^{(0)}(\boldsymbol{x})ds\,d\Omega + \langle s\rangle Q(\boldsymbol{x}).\end{aligned} \tag{5.21}$$

Thus, using the fact that $\int_0^\infty q(\boldsymbol{\Omega},s)ds = 1$ and $\int_0^\infty s^m q(\boldsymbol{\Omega},s)ds = s_\Omega^m(\boldsymbol{\Omega})$, we can rewrite Eq. (5.21) as:

$$\begin{aligned}\frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(\frac{s_\Omega^2(\boldsymbol{\Omega})}{2}[\boldsymbol{\Omega}\cdot\nabla]^2 - s_\Omega(\boldsymbol{\Omega})[\boldsymbol{\tau}(\boldsymbol{\Omega})\cdot\nabla][\boldsymbol{\Omega}\cdot\nabla]\right)\Phi^{(0)}(\boldsymbol{x})d\Omega \\ -\frac{(1-c)}{\langle s\rangle}\Phi^{(0)}(\boldsymbol{x}) + Q(\boldsymbol{x}) = 0.\end{aligned} \tag{5.22}$$

If we write $\boldsymbol{\tau}(\boldsymbol{\Omega}) = (\tau_x(\boldsymbol{\Omega}),\tau_y(\boldsymbol{\Omega}),\tau_z(\boldsymbol{\Omega}))$, this equation is equivalent to:

$$\begin{aligned}-\left[D_{xx}\frac{\partial^2}{\partial x^2} + D_{yy}\frac{\partial^2}{\partial y^2} + D_{zz}\frac{\partial^2}{\partial z^2} + D_{xy}\frac{\partial^2}{\partial x\partial y} + D_{xz}\frac{\partial^2}{\partial x\partial z} + D_{yz}\frac{\partial^2}{\partial y\partial z}\right]\Phi^{(0)}(\boldsymbol{x}) \\ + \frac{1-c}{\langle s\rangle}\Phi^{(0)}(\boldsymbol{x}) = Q(\boldsymbol{x}),\end{aligned} \tag{5.23}$$

where $D_{xx}, D_{yy}, D_{zz}, D_{xy}, D_{xz},$ and D_{yz} are the diffusion coefficients given by

$$D_{xx} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(\frac{s_\Omega^2(\boldsymbol{\Omega})}{2}\Omega_x - s_\Omega(\boldsymbol{\Omega})\tau_x(\boldsymbol{\Omega})\right)\Omega_x\,d\Omega, \tag{5.24a}$$

$$D_{yy} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(\frac{s_\Omega^2(\boldsymbol{\Omega})}{2}\Omega_y - s_\Omega(\boldsymbol{\Omega})\tau_y(\boldsymbol{\Omega})\right)\Omega_y\,d\Omega, \tag{5.24b}$$

$$D_{zz} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(\frac{s_\Omega^2(\boldsymbol{\Omega})}{2}\Omega_z - s_\Omega(\boldsymbol{\Omega})\tau_z(\boldsymbol{\Omega})\right)\Omega_z\,d\Omega, \tag{5.24c}$$

$$D_{xy} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(s_\Omega^2(\boldsymbol{\Omega})\Omega_x\Omega_y - s_\Omega(\boldsymbol{\Omega})[\tau_x(\boldsymbol{\Omega})\Omega_y + \tau_y(\boldsymbol{\Omega})\Omega_x]\right)d\Omega, \tag{5.24d}$$

$$D_{xz} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(s_\Omega^2(\boldsymbol{\Omega})\Omega_x\Omega_z - s_\Omega(\boldsymbol{\Omega})[\tau_x(\boldsymbol{\Omega})\Omega_z + \tau_z(\boldsymbol{\Omega})\Omega_x]\right)d\Omega, \tag{5.24e}$$

$$D_{yz} = \frac{1}{4\pi\langle s\rangle}\int_{4\pi}\left(s_\Omega^2(\boldsymbol{\Omega})\Omega_y\Omega_z - s_\Omega(\boldsymbol{\Omega})[\tau_y(\boldsymbol{\Omega})\Omega_z + \tau_z(\boldsymbol{\Omega})\Omega_y]\right)d\Omega. \tag{5.24f}$$

Summarizing: the solution $\psi(\boldsymbol{x},\boldsymbol{\Omega},s)$ of Eq. (5.4) satisfies:

$$\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{\Phi^{(0)}(\boldsymbol{x})}{4\pi}\frac{e^{-\int_0^s\Sigma_t(\boldsymbol{\Omega},s')ds'}}{\langle s\rangle} + O(\varepsilon), \tag{5.25}$$

where $\Phi^{(0)}(\boldsymbol{x})$ satisfies Eq. (5.23). Integrating Eq. (5.25) over $0 < s < \infty$ and using Eq. (3.16), we obtain an expression to the classic angular flux (to leading order):

$$\psi_c(\boldsymbol{x},\boldsymbol{\Omega}) = \Phi^{(0)}(\boldsymbol{x})\frac{s_\Omega(\boldsymbol{\Omega})}{4\pi\langle s\rangle}. \tag{5.26}$$

5.1. Special case 1: isotropic scattering

In the case of isotropic scattering, $P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}') = 1/4\pi$ and

$$\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}) = -\frac{1}{4\pi}\int_{4\pi}\boldsymbol{\Omega}'\,s_\Omega(\boldsymbol{\Omega}')d\Omega' = 0, \tag{5.27}$$

since $s_\Omega(\boldsymbol{\Omega})$ is an even function of $\boldsymbol{\Omega}$. Introducing this result into Eqs. (5.17), we obtain $\boldsymbol{\tau}_n(\boldsymbol{\Omega}) = 0\ \forall n \geqslant 0$. Hence, by Eq. (5.16), $\boldsymbol{\tau}(\boldsymbol{\Omega}) = 0$, and Eqs. (5.24) can be writen as

$$D_{xx} = \frac{1}{2\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}s_\Omega^2(\boldsymbol{\Omega})\Omega_x^2\,d\Omega\right), \tag{5.28a}$$

$$D_{yy} = \frac{1}{2\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}s_\Omega^2(\boldsymbol{\Omega})\Omega_y^2\,d\Omega\right), \tag{5.28b}$$

$$D_{zz} = \frac{1}{2\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}s_\Omega^2(\boldsymbol{\Omega})\Omega_z^2\,d\Omega\right), \tag{5.28c}$$

$$D_{xy} = \frac{1}{\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}s_\Omega^2(\boldsymbol{\Omega})\Omega_x\Omega_y\,d\Omega\right), \tag{5.28d}$$

$$D_{xz} = \frac{1}{\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}s_\Omega^2(\boldsymbol{\Omega})\Omega_x\Omega_z\,d\Omega\right), \tag{5.28e}$$

$$D_{yz} = \frac{1}{\langle s\rangle}\left(\frac{1}{4\pi}\int_{4\pi}s_\Omega^2(\boldsymbol{\Omega})\Omega_y\Omega_z\,d\Omega\right). \tag{5.28f}$$

5.2. Special case 2: isotropic scattering and azimuthal symmetry

A general diffusion equation with no off-diagonal terms (that is, without diffusion coefficients that depend on more than one direction) can be obtained in systems with azimuthal symmetry (such as in PBR problems). Specifically, if we define the polar angle against the z-axis such that $(\Omega_x, \Omega_y, \Omega_z) = \left(\sqrt{1-\mu^2}\cos\varphi, \sqrt{1-\mu^2}\sin\varphi, \mu\right)$, the probability distribution function for distance-to-collision is independent of the azimuthal angle φ; that is, $s^m_{\boldsymbol{\Omega}}(\boldsymbol{\Omega}) = s^m_{\boldsymbol{\Omega}}(\mu)$ depends only upon the polar angle μ. Then, $D_{xy} = D_{xz} = D_{yz} = 0$ and $D_{xx} = D_{yy}$, and we obtain the following anisotropic diffusion equation for $\Phi^{(0)}(\boldsymbol{x})$:

$$-D_{xx}\frac{\partial^2}{\partial x^2}\Phi^{(0)}(\boldsymbol{x}) - D_{yy}\frac{\partial^2}{\partial y^2}\Phi^{(0)}(\boldsymbol{x}) - D_{zz}\frac{\partial^2}{\partial z^2}\Phi^{(0)}(\boldsymbol{x}) + \frac{1-c}{\langle s\rangle}\Phi^{(0)}(\boldsymbol{x}) = Q(\boldsymbol{x}), \tag{5.29}$$

where $D_{xx} = D_{yy}$ are given by Eq. (5.28a) = Eq. (5.28b), and D_{zz} is given by Eq. (5.28c).

5.3. Special case 3: standard GLBE ($\Sigma_t(\boldsymbol{\Omega}, s) = \Sigma_t(s)$)

Let us now examine the situation in which the locations of the scattering centers are correlated but independent of direction. In this case, we can write $\Sigma_t(\boldsymbol{\Omega}, s) = \Sigma_t(s)$, and Eq. (3.7) yields $q(\boldsymbol{\Omega}, s) = \Sigma_t(s)e^{-\int_0^s \Sigma_t(s')ds'}$. Introducing this result into Eq. (3.16), we see that $s_{\boldsymbol{\Omega}}(\boldsymbol{\Omega}) = s_{\boldsymbol{\Omega}}$ is now independent of $\boldsymbol{\Omega}$, and we can use Eq. (3.18) to obtain $\langle s\rangle = s_{\boldsymbol{\Omega}}$. (Similarly, $s^2_{\boldsymbol{\Omega}}(\boldsymbol{\Omega}) = \langle s^2\rangle$.) Therefore, operating on Eq. (5.26) by $\int_{4\pi}(\cdot)d\Omega$, we obtain

$$\int_{4\pi}\psi_c(\boldsymbol{x}, \boldsymbol{\Omega})d\Omega = \Phi^{(0)}(\boldsymbol{x}). \tag{5.30}$$

Thus, the solution $\Phi^{(0)}(\boldsymbol{x})$ of Eq. (5.23) is the classic scalar flux (to leading order). Furthermore, we can write

$$\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}) = -\int_{4\pi}\boldsymbol{\Omega}'P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')s_{\boldsymbol{\Omega}}(\boldsymbol{\Omega}')d\Omega' = -\langle s\rangle\int_{4\pi}\boldsymbol{\Omega}'P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')d\Omega'. \tag{5.31a}$$

To evaluate this integral, we choose the system of coordinates such that $\boldsymbol{\Omega} = (0,0,1) = \vec{\boldsymbol{k}}$. Then, $\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}' = \mu'$ and

$$\int_{4\pi}\boldsymbol{\Omega}'P^*(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')d\Omega' = 2\pi\vec{\boldsymbol{k}}\int_{-1}^{1}\mu'P^*(\mu')d\mu' = 2\pi\boldsymbol{\Omega}\int_{-1}^{1}\mu'P^*(\mu')d\mu'. \tag{5.31b}$$

We know (Lewis and Miller, 1993) that $P_1(\mu') = \mu'$; thus, using Eqs. (5.3):

$$\int_{-1}^{1}\mu'P^*(\mu')d\mu' = \int_{-1}^{1}\frac{3}{4\pi}a_1^*\mu'^2d\mu' = \frac{a_1^*}{2\pi} = \frac{ca_1}{2\pi}, \tag{5.31c}$$

due to the orthogonality of the Legendre polynomials. Since $a_1 = \bar{\mu}_0$ (the mean scattering cosine), Eqs. (5.31) yield the explicit expression

$$\widehat{\boldsymbol{S}}(\boldsymbol{\Omega}) = -\langle s\rangle\left(2\pi\boldsymbol{\Omega}\frac{c\bar{\mu}_0}{2\pi}\right) = -\langle s\rangle\ \boldsymbol{\Omega}[c\bar{\mu}_0]. \tag{5.32}$$

Introducing this equation into Eqs. (5.17), we obtain $\boldsymbol{\tau}_n(\boldsymbol{\Omega}) = -\langle s\rangle\ \boldsymbol{\Omega}[c\bar{\mu}_0]^{n+1}\ \forall n \geqslant 0$; and using Eq. (5.16):

$$\boldsymbol{\tau}(\boldsymbol{\Omega}) = -\frac{c\bar{\mu}_0}{1-c\bar{\mu}_0}\ \langle s\rangle\ \boldsymbol{\Omega}. \tag{5.33}$$

In this case, the angular integrals in Eqs. (5.24) yield:

$$D = D_{xx} = D_{yy} = D_{zz} = \frac{1}{3}\left(\frac{\langle s^2\rangle}{2\langle s\rangle} + \frac{c\bar{\mu}_0}{1-c\bar{\mu}_0}\langle s\rangle\right), \tag{5.34a}$$

$$D_{xy} = D_{xz} = D_{yz} = 0, \tag{5.34b}$$

which reduces Eq. (5.23) to the result obtained in Larsen (2007).

Note: if $q(\boldsymbol{\Omega}, s)$ were to decay algebraically as $s\longrightarrow\infty$ as:

$$q(\boldsymbol{\Omega}, s) \geqslant \frac{\text{constant}}{s^3} \quad \text{for} \quad s \geqslant 1, \tag{5.35}$$

then the asymptotic diffusion approximation developed here would be invalid, since this would imply

$$s^2_{\boldsymbol{\Omega}}(\boldsymbol{\Omega}) = \int_0^\infty s^2 q(\boldsymbol{\Omega}, s)ds = \infty. \tag{5.36}$$

The asymptotic analysis tacitly requires both $s_{\boldsymbol{\Omega}}$ and $s^2_{\boldsymbol{\Omega}}$ to be finite. Physically, when $s^2_{\boldsymbol{\Omega}} = \infty$, particles will travel large distances between collisions too often. That is, sufficiently long flight paths will occur sufficiently often that the diffusion description developed here becomes invalid. Following the nomenclature in Davis (2008), standard diffusion ($s^2_{\boldsymbol{\Omega}} < \infty$) is an asymptotic approximation of the GLBE, while anomalous diffusion ($s^2_{\boldsymbol{\Omega}} = \infty$) is not.

6. Reduction to the classic theory

We now show that, with the classic assumption that the locations of the scattering centers are uncorrelated and do not depend upon direction, the results obtained by the GLBE presented here reduce to the results of the classic theory. In other words, we now assume that

$$\Sigma_t(\boldsymbol{\Omega}, s) = \Sigma_t \equiv \text{constant}. \tag{6.1}$$

In this case, Eq. (2.4) can be rewritten as

$$\frac{\partial\psi}{\partial s}(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \boldsymbol{\Omega}\cdot\nabla\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) + \Sigma_t\psi(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \delta(s)\ \Sigma_s\int_{4\pi}\int_0^\infty P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\psi(\boldsymbol{x}, \boldsymbol{\Omega}', s')ds'd\Omega' + \delta(s)\frac{Q(\boldsymbol{x})}{4\pi}, \tag{6.2}$$

where $\Sigma_s = c\Sigma_t$. Operating on this equation by $\int_{-\varepsilon}^\infty(\cdot)ds$ and using Eq. (2.8), we obtain

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}, \infty) - \psi(\boldsymbol{x}, \boldsymbol{\Omega}, -\varepsilon) + \boldsymbol{\Omega}\cdot\nabla\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}) + \Sigma_t\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}) = \Sigma_s\int_{4\pi}P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x})}{4\pi}. \tag{6.3}$$

Using the fact that $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, \infty) = \psi(\boldsymbol{x}, \boldsymbol{\Omega}, -\varepsilon) = 0$, we have

$$\boldsymbol{\Omega}\cdot\nabla\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}) + \Sigma_t\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}) = \Sigma_s\int_{4\pi}P(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\psi_c(\boldsymbol{x}, \boldsymbol{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x})}{4\pi}, \tag{6.4}$$

which is, of course, the classic linear Boltzmann equation.

Moreover, if Eq. (6.1) holds, then Eq. (3.7) yields

$$q(\boldsymbol{\Omega}, s) = \Sigma_t e^{-\Sigma_t s} = p(s); \tag{6.5}$$

that is, the probability distribution function for distance-to-collision is given by an exponential. Introducing Eq. (6.5) into Eq. (3.16), we can use Eq. (3.18) to obtain

$$\langle s\rangle = s_{\boldsymbol{\Omega}}(\boldsymbol{\Omega}) = \frac{1}{\Sigma_t}, \tag{6.6a}$$

which is the classic expression for the mean free path. Also, the mean-squared free path is given by:

$$\langle s^2\rangle = s^2_{\boldsymbol{\Omega}}(\boldsymbol{\Omega}) = \int_0^\infty s^2 p(s)ds = \frac{2}{\Sigma_t^2}. \tag{6.6b}$$

For the integral formulation, Eqs. (4.10) can now be easily reduced to their classic form, since Eq. (6.1) allows us to write

$$\hat{q}(|\boldsymbol{x}-\boldsymbol{x}'|) = \Sigma_t e^{-\Sigma_t|\boldsymbol{x}-\boldsymbol{x}'|} \tag{6.7}$$

in Eq. (4.10a). Furthermore, Eq. (4.1) yields

$$f(\boldsymbol{x},\boldsymbol{\Omega}) = \Sigma_t \int_0^\infty \psi(\boldsymbol{x},\boldsymbol{\Omega},s)ds = \Sigma_t\psi_c(\boldsymbol{x},\boldsymbol{\Omega}), \tag{6.8}$$

and thus by Eq. (4.11b),

$$\widehat{F}(\boldsymbol{x}) = \Sigma_t \int_{4\pi} \psi_c(\boldsymbol{x},\boldsymbol{\Omega}')d\Omega' = \Sigma_t\phi_c(\boldsymbol{x}). \tag{6.9}$$

Using Eq. (6.7) and the previous result in Eqs. (4.12b) and (4.12c), we obtain:

$$\psi_c(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{1}{4\pi}\int_0^\infty [\Sigma_s\phi_c(\boldsymbol{x}-s\boldsymbol{\Omega}) + Q(\boldsymbol{x}-s\boldsymbol{\Omega})]e^{-\Sigma_t s}\,ds, \tag{6.10a}$$

and

$$\phi_c(\boldsymbol{x}) = \iiint [\Sigma_s\phi_c(\boldsymbol{x}') + Q(\boldsymbol{x}')]\frac{e^{-\Sigma_t|\boldsymbol{x}-\boldsymbol{x}'|}}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|^2}\,dV'. \tag{6.10b}$$

Eq. (6.10b) is the classic integral transport equation for the scalar flux $\phi_c(\boldsymbol{x})$, and Eq. (6.10a) is the classic expression for the angular flux $\psi_c(\boldsymbol{x},\boldsymbol{\Omega})$ in terms of $\phi_c(\boldsymbol{x})$, for the case of isotropic scattering.

For the theory involving the asymptotic diffusion limit, if Eq. (6.1) holds, then we can use Eqs. (5.34) and (6.6) to reduce Eq. (5.23) to the classic diffusion expression:

$$-\frac{1}{3\Sigma_t(1-c\bar{\mu}_0)}\nabla^2\Phi^{(0)}(\boldsymbol{x}) + \Sigma_t(1-c)\Phi^{(0)}(\boldsymbol{x}) = Q(\boldsymbol{x}). \tag{6.11}$$

In short, we have shown that when Eq. (6.1) holds, the new generalized theory reduces to the classic transport theory, as it must.

7. Discussion

We have generalized the theory introduced in Larsen (2007), in which the true non-exponential probability distribution function for the distance-to-collision is replaced by its ensemble average. This ensemble-averaged probability distribution function is used at all points to determine how far particles travel between collisions. The original aspect of the present model is in allowing the cross sections of the homogenized system to be functions of both angle $\boldsymbol{\Omega}$ and distance-to-collision s; that is, we assume that the locations of the scattering centers are correlated *and* depend upon direction.

With this method, we obtain a new generalized Boltzmann equation that preserves all relevant asymptotic limits and reduces to the classic Boltzmann equation in the case of a homogeneous system. The disadvantage is that there is no simple way to obtain expressions for these s-dependent cross sections; they need to be numerically estimated. Nevertheless, we use this result to develop a generalized diffusion equation, which does not depend upon the variable s, but rather on its mean and mean-squared values s_Ω and s^2_Ω. The diffusion approximation also preserves all relevant limits and reduces to classic diffusion in homogeneous systems. Moreover, it yields anisotropic diffusion coefficients when the locations of the scattering centers depend upon direction.

The present theory requires more information about a random system than the atomic mix method; if a random system is diffusive, then only s_Ω and s^2_Ω need to be estimated (for isotropic diffusion, they will not depend on $\boldsymbol{\Omega}$). This extra information is microscopic in nature; it is not a closure relation, as in the Levermore–Pomraning method. Our theory uses this microscopic data in a generalized Boltzmann equation or in a generalized diffusion equation to determine approximate mean macroscopic quantities. In Part II of this paper (Vasques and Larsen, 2014) we numerically show that, for problems of the pebble bed kind, this new approach accurately predicts the anisotropic behavior of the systems, which cannot be achieved by the standard GLBE and the classic approaches currently in use.

In the future, we intend to extend the present work to problems with inhomogeneous statistics, as well as for energy-dependent systems. Also, having developed a theory for the mean flux of particles, the next logical step is to try to develop a similar theory that is capable of calculating variance; this is another of our goals.

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