Journal of Quantitative Spectroscopy & Radiative Transfer 189 (2017) 133–148

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

# Benchmark solutions for transport in *d*-dimensional Markov binary mixtures

Coline Larmier, François-Xavier Hugot, Fausto Malvagi, Alain Mazzolo, Andrea Zoia*

*Den-Service d'Etudes des Réacteurs et de Mathématiques Appliquées (SERMA), CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, FRANCE*

A R T I C L E I N F O

*Article history:*
Received 9 September 2016
Received in revised form
14 November 2016
Accepted 16 November 2016
Available online 25 November 2016

*Keywords:*
Markov geometries
Benchmark
Monte Carlo
Tripoli-4®

A B S T R A C T

Linear particle transport in stochastic media is key to such relevant applications as neutron diffusion in randomly mixed immiscible materials, light propagation through engineered optical materials, and inertial confinement fusion, only to name a few. We extend the pioneering work by Adams, Larsen and Pomraning [1] (recently revisited by Brantley [2]) by considering a series of benchmark configurations for mono-energetic and isotropic transport through Markov binary mixtures in dimension *d*. The stochastic media are generated by resorting to Poisson random tessellations in 1*d* slab, 2*d* extruded, and full 3*d* geometry. For each realization, particle transport is performed by resorting to the Monte Carlo simulation. The distributions of the transmission and reflection coefficients on the free surfaces of the geometry are subsequently estimated, and the average values over the ensemble of realizations are computed. Reference solutions for the benchmark have never been provided before for two- and three-dimensional Poisson tessellations, and the results presented in this paper might thus be useful in order to validate fast but approximated models for particle transport in Markov stochastic media, such as the celebrated Chord Length Sampling algorithm.



## 1. Introduction

Linear transport through heterogeneous and disordered media emerges in several applications in nuclear science and engineering. Examples are widespread and concern for instance neutron diffusion in pebble-bed reactors [3] or randomly mixed immiscible materials [4,5], and inertial confinement fusion [6–8]. Besides, the spectrum of applications is fairly broad and far reaching [9,10], and concerns also light propagation through engineered optical materials [11–13] or turbid media [14–16], tracer diffusion in biological tissues [17], and radiation trapping in hot atomic vapours [18], only to name a few. The key goal of particle transport theory in stochastic media consists in deriving a formalism for the description of the ensemble-averaged angular particle flux $\langle \varphi(\mathbf{r},\boldsymbol{\omega})\rangle$, where $\varphi(\mathbf{r},\boldsymbol{\omega})$ solves the linear Boltzmann equation

$$\boldsymbol{\omega}\cdot\nabla\varphi + \Sigma(\mathbf{r})\varphi = \int \Sigma_s(\boldsymbol{\omega}'\to\boldsymbol{\omega},\mathbf{r})\varphi(\mathbf{r},\boldsymbol{\omega}')d\boldsymbol{\omega}' + S, \tag{1}$$

$\mathbf{r}$ and $\boldsymbol{\omega}$ denoting the position and direction variables, respectively, $\Sigma(\mathbf{r})$ being the total cross section, $\Sigma_s(\boldsymbol{\omega}'\to\boldsymbol{\omega},\mathbf{r})$ the differential scattering cross section, and $S = S(\mathbf{r},\boldsymbol{\omega})$ the source term. For isotropic scattering, the differential scattering cross section simplifies to $\Sigma_s(\boldsymbol{\omega}'\to\boldsymbol{\omega},\mathbf{r}) = \Sigma_s(\mathbf{r})/\Omega_d$, where $\Omega_d$ is the surface of the unit sphere in dimension *d*. For the sake of simplicity, we have here focused our attention to the case of mono-energetic transport in non-fissile media, in stationary (i.e., time-independent) conditions. However, these hypotheses are not restrictive (see the discussion in [4]). The stochastic nature of particle transport stems from the materials composing the traversed medium being randomly distributed according to some statistical law. Hence, the quantities $\Sigma(\mathbf{r})$, $\Sigma_s(\boldsymbol{\omega}'\to\boldsymbol{\omega},\mathbf{r})$ and $S(\mathbf{r},\boldsymbol{\omega})$ are in principle random variables.

A physical realization of the system under analysis will be denoted by a state *q*, associated to some stationary probability $\mathcal{P}(q)$ of observing the state *q*. To each state *q* thus correspond the functions $\Sigma^{(q)}(\mathbf{r})$, $\Sigma_s^{(q)}(\boldsymbol{\omega}'\to\boldsymbol{\omega},\mathbf{r})$ and $S^{(q)}(\mathbf{r},\boldsymbol{\omega})$ for the material properties [5,4]. The ensemble-averaged angular flux is then formally defined as

$$\langle \varphi(\mathbf{r},\boldsymbol{\omega})\rangle = \int \mathcal{P}(q)\varphi^{(q)}(\mathbf{r},\boldsymbol{\omega})dq, \tag{2}$$

where $\varphi^{(q)}(\mathbf{r},\boldsymbol{\omega})$ is the solution of the Boltzmann Eq. (1) corresponding to a single realization *q*. The ensemble-averaged angular flux can be decomposed as

$$\langle \varphi(\mathbf{r},\boldsymbol{\omega})\rangle = \sum_i p_i(\mathbf{r})\langle \varphi_i(\mathbf{r},\boldsymbol{\omega})\rangle, \tag{3}$$

where $p_i(\mathbf{r}) = \int \mathcal{P}(q)\chi_i(\mathbf{r})dq$ is the probability of finding the

* Corresponding author.
*E-mail address:* andrea.zoia@cea.fr (A. Zoia).

http://dx.doi.org/10.1016/j.jqsrt.2016.11.015
0022-4073/

material of index $i$ at position $\mathbf{r}$ (we denote by $\chi_i(\mathbf{r})$ the marker function of material $i$ at position $\mathbf{r}$), and $\langle\varphi_i(\mathbf{r},\boldsymbol{\omega})\rangle$ is restricted to those realizations that have material $i$ at position $\mathbf{r}$:

$$p_i(\mathbf{r})\langle\varphi_i(\mathbf{r},\boldsymbol{\omega})\rangle = \int \mathcal{P}(q)\chi_i(\mathbf{r})\varphi^{(q)}(\mathbf{r},\boldsymbol{\omega})dq. \tag{4}$$

A widely adopted model of random media is the so-called binary stochastic mixing, where only two immiscible materials (say $\alpha$ and $\beta$) are present [4]. Then, by averaging Eq. (1) over realizations having material $\alpha$ at $\mathbf{r}$, we obtain the following equation for $\langle\varphi_\alpha(\mathbf{r},\boldsymbol{\omega})\rangle$

$$\left[\boldsymbol{\omega}\cdot\nabla + \Sigma_\alpha\right]p_\alpha\langle\varphi_\alpha\rangle = \frac{p_\alpha\Sigma_{s,\alpha}}{\Omega_d}\int\langle\varphi_\alpha(\mathbf{r},\boldsymbol{\omega}')\rangle d\boldsymbol{\omega}' + p_\alpha S_\alpha + U_{\alpha,\beta}, \tag{5}$$

where

$$U_{\alpha,\beta} = p_{\beta,\alpha}\langle\varphi_{\beta,\alpha}\rangle - p_{\alpha,\beta}\langle\varphi_{\alpha,\beta}\rangle, \tag{6}$$

with $p_{i,j} = p_{i,j}(\mathbf{r},\boldsymbol{\omega})$ denoting the probability per unit length of crossing the interface from material $i$ to material $j$ for a particle located at $\mathbf{r}$ and travelling in direction $\boldsymbol{\omega}$, and $\langle\varphi_{i,j}\rangle$ denoting the angular flux averaged over those realizations where there is a transition from material $i$ to material $j$ for a particle located at $\mathbf{r}$ and travelling in direction $\boldsymbol{\omega}$. The cross sections $\Sigma_\alpha$ and $\Sigma_{s,\alpha}$ are those of material $\alpha$. The equation for $\langle\varphi_\beta(\mathbf{r},\boldsymbol{\omega})\rangle$ is immediately obtained from Eq. (5) by permuting the indexes $\alpha$ and $\beta$.

The set of equations in Eq. (5) (whose derivation contains no approximations so far) can be shown to form an infinite hierarchy, since the terms $\langle\varphi_\alpha\rangle$ in Eq. (6) would involve equations for the conditional averages $\langle\varphi_{\beta,\alpha}\rangle$ and $\langle\varphi_{\alpha,\beta}\rangle$, which in turn would further involve additional conditional averages [4,5]. Generally speaking, it is necessary to truncate the infinite set of equations with some appropriate model leading to a closure formula, depending on the underlying mixing statistics. The celebrated Levermore-Pomraning model assumes for instance $\langle\varphi_{\alpha,\beta}\rangle = \langle\varphi_\alpha\rangle$ for homogeneous Markov mixing statistics [4,19], which is defined by

$$p_{i,j}(\mathbf{r},\boldsymbol{\omega}) = \frac{p_i}{\Lambda_i(\boldsymbol{\omega})}, \tag{7}$$

depending on the starting position alone, where $\Lambda_i(\boldsymbol{\omega})$ is the mean chord length for trajectories crossing material $i$ in direction $\boldsymbol{\omega}$. Several generalisations of this model have been later proposed, including higher-order closure schemes [4,20]. In parallel, Monte Carlo algorithms such as the Chord Length Sampling have been conceived in order to formally solve the Levermore-Pomraning model, and have been further extended so as to include partial memory effects due to correlations for particles crossing back and forth the same materials [6,7]. Their common feature is that they allow a simpler, albeit approximate, treatment of transport in stochastic mixtures, which might be convenient in practical applications where a trade-off between computational time and precision can be worth considering. Originally formulated for Markov statistics, these models have been largely applied also to random inclusions of disks or spheres into background matrices, with application to pebble-bed and very high temperature gas-cooled reactors [21,22].

In order to assess the accuracy of the various approximate models it is therefore mandatory to compute reference solutions for the exact Eqs. (5). Such solutions can be obtained in the following way: first, a realization of the medium is sampled from the underlying mixing statistics; then, the linear transport equations corresponding to this realization are solved by either deterministic or Monte Carlo methods, and the physical observables of interest are determined; this procedure is repeated several times so as to create a sufficiently large collection of realizations, and ensemble averages are finally taken for the physical observables. For this purpose, a number of benchmark problems for Markov mixing have been proposed in the literature so far [1,5,2,23–25], with focus exclusively on $1d$ geometries, either of the rod or slab type.

The aim of this work is two-fold. First, we will revisit the classical benchmark problem proposed by Adams, Larsen and Pomraning for transport in stochastic media [1]. We will present reference solutions obtained by Monte Carlo particle transport simulation through $1d$ slab, $2d$ extruded and $3d$ tessellations of a finite-size box with Markov mixing. We will compute the particle flux $\langle\varphi\rangle$, the transmission coefficient $\langle T\rangle$ and the reflection coefficient $\langle R\rangle$ by taking ensemble averages over the realizations; the dispersion of the physical observables around their average values will be assessed by evaluating their full distributions. Second, we will discuss the impact of dimension on the obtained results, since benchmark solutions for transport in $2d$ extruded and $3d$ tessellations have never been addressed before [26].

This paper is organized as follows. In Section 2 we recall the benchmark specifications and set up the required notation. In Section 3 we discuss the algorithms needed in order to generate the material configurations corresponding to homogeneous Markov mixing, by resorting to the so-called colored Poisson tessellations. Then, in Section 4 we will present our simulation results for the physical observables of interest, and discuss the obtained findings. Conclusions will be finally drawn in Section 5.

## 2. Benchmark specifications

The benchmark specifications for our work are essentially taken from those originally proposed in [1] and [5], and later extended in [25,2,23,24]. We consider single-speed linear particle transport through a stochastic binary medium with homogeneous Markov mixing. The medium is non-multiplying, with isotropic scattering. The geometry consists of a cubic box of side $L=10$, with reflective boundary conditions on all sides of the box except two opposite faces (say those perpendicular to the $x$ axis), where leakage boundary conditions are imposed: particles that leave the domain through these faces can not re-enter. Lengths are expressed in arbitrary units. In [1] and [5], system sizes $L=0.1$ and $L=1$ were also considered, but in this work we will focus on the case $L=10$, which leads to more physically relevant configurations. Two kinds of non-stochastic sources will be considered: either an imposed normalized incident angular flux on the leakage surface at $x=0$ (with zero interior sources), or a distributed homogeneous and isotropic normalized interior source (with zero incident angular flux on the leakage surfaces). Following the notation in [2], the benchmark configurations pertaining to the former kind of source will be called *suite* I, whereas those pertaining to the latter will be called *suite* II. The material properties for the Markov mixing are entirely defined by assigning the average chord length for each material $i=\alpha,\beta$, namely $\Lambda_i$, which in turn allows deriving the homogeneous probability $p_i$ of finding material $i$ at an arbitrary location within the box, namely

$$p_i = \frac{\Lambda_i}{\Lambda_i + \Lambda_j}. \tag{8}$$

Note that the material probability $p_i$ defines the volume fraction for material $i$. The cross sections for each material will be denoted as customary $\Sigma_i$ for the total cross section and $\Sigma_{s,i}$ for the scattering cross section. The average number of particles surviving a collision in material $i$ will be denoted by $c_i = \Sigma_{s,i}/\Sigma_i \le 1$. The physical parameters for the benchmark configurations are recalled in Tables 1 and 2 : three cases (numbered 1, 2 and 3) are considered, each containing three sub-cases (noted $a$, $b$ and $c$). The case numbers correspond to permutation of materials, whereas the sub-cases represents varying ratios of $c_i$ for each material.