Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew
Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)

ELECTRON ENERGY DEPOSITION IN BINARY STATISTICAL MEDIA: A PDF APPROACH

Anil K. Prinja
University of New Mexico
Chemical and Nuclear Engineering Department
Albuquerque, NM 87131, USA
prinja@unm.edu

Brian C. Franke
Sandia National Laboratories
P.O. Box 5800, Albuquerque, NM 87185-1179, USA
bcfrank@sandia.gov

ABSTRACT

Energy deposition from high energy electrons in binary statistical media is considered in a probabilistic setting. A systematic method is presented for deriving an equation for the conditional probability density function of the angular flux that correctly incorporates scattering. Two closure problems are encountered: one is related to the random material transitions, for which the Levermore-Pomraning or Markovian closure model is used, and the other arises from scattering induced correlations. The latter vanishes when equations for the conditional ensemble averaged flux are considered but the equations for all higher moments remain statistically open. Numerical results for the mean dose in binary gold-air and water-air mixtures are compared against benchmark results obtained for alternating slabs with Poisson statistics. The LP-closure model for the dose yields consistently more accurate results than the atomic mix limit for the cases considered. Also, the accuracy of the closure appears to increase as scattering becomes more forward peaked, indicating that the problem appears increasingly Markovian with decreasing numbers of backward moving particles.

Key Words: Stochastic, PDF, Electron Transport, Dose

1. INTRODUCTION

The subject of neutral particle transport in binary statistical media, that is, in media comprising randomly mixed chunks of two different materials, has received much attention over the last two decades. The review by Pomraning [1] summarizes the work on this subject and provides an exhaustive list of references to earlier work. The main interest has been on developing statistically closed equations for the conditional mean angular flux $\psi_i(\vec{r}, \vec{\Omega}, t)$, conditioned upon the point $\vec{r}$ being in material type i, $i = 1, 2$, for a number of applications in neutron transport and radiative transfer. In the early work [2, 3], a purely absorbing medium was first considered and the material statistics were assumed to be Markovian with transition points following a Poisson distribution along any ray. That is, the material thicknesses were assumed to be exponentially distributed with mean chunk size given by λ_i, $i = 1, 2$. A so-called stochastic Liouville equation was postulated to describe the conditional probability density of the angular flux [4], and equations for the conditional mean angular flux were constructed by taking an appropriate flux moment. Additional terms, scaling with the mean chunk size of each material, were introduced to account for the effect of material transitions. It was argued that the model was nevertheless exact for purely absorbing media because the stochastic process represented by the angular flux and the material geometry was jointly Markovian. In fact, it can be shown from fundamental probabilistic considerations that the (differential) Chapman-Kolmogorov equation for the joint process is equivalent to the stochastic Liouville equation if the rate parameters are equated to the mean chunk sizes. Thus the model is exact, or statistically closed, for purely absorbing media when the material transitions are exponentially distributed. Moreover, the model remains valid when a statistically independent volume source is included.

The addition of scattering introduces statistical correlations between angular fluxes along different directions, in particular between particles moving in the forward and reverse hemispheres. The joint process is no longer Markovian under these conditions and a Chapman-Kolmogorov equation cannot therefore be written down [5]. An approximate model is obtained, however, by regarding the scattering source as a statistically independent source and proceeding as before to write down the appropriate stochastic Liouville equation with material coupling terms added and justified on the basis of the Markovian source assumption [3]. Averaging then yields a statistically closed pair of transport equations for the conditional angular fluxes in each material, including scattering. As derived, the equations for the conditional mean angular fluxes are approximate for two related reasons: the use of the Markovian form of the material transition terms, known in the literature as the Markovian closure or the Levermore-Pomraning (LP-) closure, and the apparent neglect of correlations between the scattering source and the angular flux. Nevertheless, this so-called standard model has found widespread use in the work to date on transport in binary statistical media.

In a different approach [6], equations for the conditional mean fluxes are derived directly by conditionally averaging the transport equation written down for individual material geometry realizations. That is, no appeal was made to an explicit probabilistic model such as the stochastic Liouville equation used in the original work. This approach is systematic and the effect of material transitions appears explicitly in the form of conditional mean interface angular fluxes, that is, fluxes averaged over realizations such that the point in question is an interface between the two materials. If the Markovian or LP-closure is used to relate these interface fluxes to the interior mean fluxes, the standard model with scattering is immediately realized. Notably, this is achieved without any restrictions on the scattering source, seemingly in contrast to the previous explicitly probabilistic approach, and has fueled speculation that correlations between the angular fluxes introduced by scattering are in some sense irrelevant [3]. This issue has not been satisfactorily resolved in spite of the extensive application of the standard model.

In this article we present an approach which reconciles the apparently conflicting conclusions on the role of scattering in the two heuristic approaches discussed above and, furthermore, we extend the methodology to describe charged particle transport in random media. Specifically, we present a first principles derivation of kinetic equations for the one-point joint probability density function (PDF) of the electron angular flux and the material geometry, explicitly incorporating scattering and continuous slowing down (CSD) interactions. We adapt an approach originating in the kinetic theory of gases [7, 8], but which is also employed in stochastic formulations of fluid turbulence [9, 10] and in statistical physics [11]. Our approach leads to two closure problems: one due to material transitions, mirroring that encountered in the heuristic derivations, and the other due to the fundamentally non-Markovian nature of scattering but which, interestingly, is absent when equations for the conditional means only are considered.

Without loss of generality, a binary random material mix is assumed but the statistics of the mix are initially left unspecified. The LP-closure is then applied to obtain a coupled set of transport equations for the conditional mean electron angular fluxes. For CSD energy loss without scattering, the model is exact if the material statistics are Poissonian, otherwise the model represents an approximation. Numerical results for the unconditional mean dose are obtained by Monte Carlo simulation of the process, with and without scattering, and contrasted against predictions from the simpler atomic mix model. Corresponding benchmark results, to test the accuracy of the LP-closure for high energy charged particles, are also obtained by Monte Carlo simulation for 1D alternating slabs with Poisson mixing statistics. While our stochastic model gives equations for higher order moments, these are unclosed when scattering is present, and while we can speculate on synthetic closures for the scattering source, we have not tested these numerically as yet. However, we do present benchmark results from the numerical experiments for the standard deviation in the dose profile as well as the complete pdf of the dose at selected spatial locations.

2. THE PDF APPROACH FOR ELECTRON TRANSPORT

We consider electron transport in a random mixture of two immiscible materials, labeled 1 and 2. It is not necessary to a priori specify the material statistics in our approach, but a specific statistical model for the geometry will be employed later to justify a closure and for generating benchmark results. We restrict considerations to time independent material transitions, although this is not essential and can be readily incorporated into our methodology. For a given realization of the geometry the angular flux of electrons $\Psi(\vec{r}, E, \vec{\Omega}, t)$ satisfies the following transport equation,

$$\frac{1}{v}\frac{\partial \Psi}{\partial t} + \vec{\Omega}\cdot\nabla\Psi - \frac{\partial}{\partial E}\left[S(\vec{r},E)\,\Psi\right] + \sigma_s(\vec{r},E)\,\Psi = \int_{4\pi} \sigma_s(\vec{r},E,\vec{\Omega}\cdot\vec{\Omega}')\,\Psi(\vec{r},E,\vec{\Omega}',t)d\vec{\Omega}', \qquad (1)$$

with the following initial and boundary conditions,

$$\Psi(\vec{r},E,\vec{\Omega},0) = \Lambda(\vec{r},E,\vec{\Omega}), \qquad (2)$$

$$\Psi(\vec{r_s},E,\vec{\Omega},t) = \Gamma(\vec{r_s},E,\vec{\Omega},t), \quad \vec{n}\cdot\vec{\Omega} < 0, \qquad (3)$$

where in Eq.(1) $\sigma_s(\vec{r},E)$ is the total electron scattering cross section, $\sigma_s(\vec{r},E,\vec{\Omega}\cdot\vec{\Omega}')$ is the differential scattering cross section and $S(\vec{r},E)$ the material stopping power. A source-free medium has been assumed here without loss of generality. A volume source, stochastic or deterministic, can be readily incorporated into the methodology to be described below. Standard assumptions for electron transport are made, namely, angular deflections without energy loss, and energy loss in the CSD approximation without deflection. These are physical approximations valid for high energy electrons and do not represent a limitation of the statistical model developed below. The initial and boundary data, $\Lambda(\vec{r},E,\vec{\Omega})$ and $\Gamma(\vec{r_s},E,\vec{\Omega},t)$, are assumed to be deterministic or, if random, to be independent of the material statistics.

The material randomness is reflected in the spatial dependence of the physical properties, namely, the cross section and the stopping power. Equation (1) then constitutes a stochastic integro-partial differential equation and its solution for different realizations of the material geometry generates a stochastic process for the angular flux. The range of possible flux values $\{\psi,\ 0<\psi<\infty\}$ in a given phase space volume is referred to as an ensemble and describes the sample space for this process. For a fixed realization we define a one-point joint micro-density $\rho(\psi,i;\vec{r},E,\vec{\Omega},t)$ such that $\rho(\cdots)\,d\psi d\vec{r}d\vec{\Omega}dE$ is the joint probability that, in the particular realization, the angular flux of electrons in $d\vec{r}$ about $\vec{r}$ travelling along direction $\vec{\Omega}$ in $d\vec{\Omega}$ with energy between E and $E+dE$ at time t lies between ψ and $\psi+d\psi$, with the point $\vec{r}$ being in material i. It is a singular quantity, or more appropriately a fine grained density, nonzero only for that value of the flux which solves the transport equation for the particular realization, and hence can be expressed as

$$\rho(\psi,i;\vec{r},E,\vec{\Omega},t) = \delta\left[\psi - \Psi(\vec{r},E,\vec{\Omega},t)\right]\,\chi_i(\vec{r}), \qquad (4)$$

where we have introduced the indicator function $\chi_i(\vec{r})$ defined such that,

$$\chi_i(\vec{r}) = \begin{cases} 1, & \text{if } i \in \text{mat}\, i \\ 0, & \text{otherwise} \end{cases} \tag{5}$$

The quantity of interest is the coarse grained density obtained upon ensemble averaging ρ over all realizations of the material statistics. We express this averaging by

$$P(\psi, i; \vec{r}, E, \vec{\Omega}, t) = \langle \rho(\psi, i; \vec{r}, E, \vec{\Omega}, t) \rangle, \tag{6}$$

where now $P(\psi, i; \vec{r}, E, \vec{\Omega}, t) d\psi d\vec{r} d\vec{\Omega} dE$ is the joint probability over the ensemble that the angular flux of electrons in $d\vec{r}$ about $\vec{r}$ travelling along direction $\vec{\Omega}$ in $d\vec{\Omega}$ with energy between E and $E + dE$ at time t lies between ψ and $\psi + d\psi$, with the point $\vec{r}$ being in material i. To make contact with previous work [3], we note that the joint density can be factored as follows

$$P(\psi, i; \vec{r}, E, \vec{\Omega}, t) = \langle \delta \left[\psi - \Psi(\vec{r}, E, \vec{\Omega}, t) \right] \mid i \rangle \, \langle \chi_i(\vec{r}) \rangle \equiv P_i(\psi; \vec{r}, E, \vec{\Omega}, t)\, p_i(\vec{r}), \tag{7}$$

where $p_i(\vec{r}) = \langle \chi_i(\vec{r}) \rangle$ is the probability that the point $\vec{r}$ lies in material i (the marginal or one-point material probability density) and $P_i(\psi; \vec{r}, E, \vec{\Omega}, t) = \langle \delta \left[\psi - \Psi(\vec{r}, E, \vec{\Omega}, t) \right] \mid i \rangle$ is the conditional probability density for the angular flux, given that, or conditioned on, $\vec{r} \in \text{mat}\, i$. We are interested in deriving an equation for this conditional density without a priori restrictions on the scattering source or on the material statistics. To proceed, we take the time derivative of the micro-density ρ to get,

$$\begin{aligned} \frac{1}{v} \frac{\partial \rho}{\partial t} &= \frac{1}{v} \frac{\partial}{\partial t} \delta \left[\psi - \Psi(\vec{r}, E, \vec{\Omega}, t) \right] \chi_i(\vec{r}) \\ &= -\frac{1}{v} \frac{\partial \Psi}{\partial t} \frac{\partial}{\partial \psi} \delta \left[\psi - \Psi(\vec{r}, E, \vec{\Omega}, t) \right] \chi_i(\vec{r}), \end{aligned} \tag{8}$$

where well known properties of the delta function have been used (this result can be verified by multiplying both sides by a test function and integrating). Inserting Eq.(1) on the right hand side of Eq.(8) gives after considerable rearrangement the following equation for the micro-density,

$$\begin{aligned} \frac{1}{v} \frac{\partial \rho}{\partial t} + \vec{\Omega} \cdot \nabla \rho - S_i \frac{\partial \rho}{\partial E} \quad + \quad & \frac{\partial S_i}{\partial E} \frac{\partial (\psi\, \rho)}{\partial \psi} - \sigma_{si} \frac{\partial (\psi\, \rho)}{\partial \psi} = \rho \frac{1}{\chi_i} \vec{\Omega} \cdot \nabla \chi_i - \\ & \frac{\partial}{\partial \psi} \int_{4\pi} d\vec{\Omega}' \int_0^\infty d\psi'\, \psi' \sigma_{si}(\vec{r}, E, \vec{\Omega} \cdot \vec{\Omega}')\, \rho_2(\psi, \psi'), \end{aligned} \tag{9}$$

where we have introduced a two-point joint density ρ_2 in the inscatter term on the right hand side, defined by

$$\rho_2(\psi, \psi', i; \vec{r}, E, \vec{\Omega}, \vec{\Omega}', t) = \delta \left[\psi - \Psi(\vec{r}, E, \vec{\Omega}, t) \right] \, \delta \left[\psi' - \Psi(\vec{r}, E, \vec{\Omega}', t) \right] \, \chi_i(\vec{r}). \tag{10}$$

Discussion of the terms on the RHS of Eq.(9), which are not in canonical form, is in order here, but we comment on them below in the context of the corresponding equation for the coarse grained conditional pdf. This may be obtained by ensemble averaging Eq.(9) and using Eq.(7), viz,

$$\begin{aligned} & \frac{1}{v} \frac{\partial}{\partial t} (p_i\, P_i) + \vec{\Omega} \cdot \nabla (p_i\, P_i) - S_i \frac{\partial}{\partial E} (p_i\, P_i) + \frac{\partial S_i}{\partial E} \frac{\partial}{\partial \psi} (\psi\, p_i\, P_i) - \sigma_{si} \frac{\partial}{\partial \psi} (\psi\, p_i\, P_i) = \\ & \langle \rho \frac{1}{\chi_i} \vec{\Omega} \cdot \nabla \chi_i \rangle - \frac{\partial}{\partial \psi} \int_{4\pi} d\vec{\Omega}' \int_0^\infty d\psi'\, \psi' \sigma_{si}(\vec{r}, E, \vec{\Omega} \cdot \vec{\Omega}')\, p_i\, P_{2i}(\psi, \psi'), \quad i = 1, 2. \end{aligned} \tag{11}$$

$P_{2i}(\psi, \psi')$ in the above equation is the conditional two-point joint density function and is related to ρ_2 as follows,

$$P_{2i}(\psi, \psi', i; \vec{r}, E, \vec{\Omega}, \vec{\Omega}', t) = \langle \delta \left[\psi - \Psi(\vec{r}, E, \vec{\Omega}, t) \right] \, \delta \left[\psi' - \Psi(\vec{r}, E, \vec{\Omega}', t) \right] \mid i \rangle. \tag{12}$$

As it stands, Eq.(11), while exact, is formal because it is stochastically open in two respects. First, the conditional two-point joint density appearing in the second term on the RHS is a higher order probability density function that describes scattering induced correlations between angular fluxes along different directions. To make this equation useful, it is necessary to either express P_{2i} explicitly in terms of P_i, i.e., invoke a closure, or to derive an equation for P_{2i} itself using the method outlined above. As can be readily anticipated, such an equation will involve still higher order correlations and therefore not eliminate the closure problem. In fact, an infinite hierarchy of successively higher order pdfs will be generated with this procedure, reminiscent of the BBGKY hierarchy in kinetic theory of gases [7, 8]. We will have more to say on this aspect of the closure problem below. The first term on the RHS of Eq.(11) also cannot be simply expressed in terms of P_i and constitutes the second closure problem. It can be readily shown that $\nabla \chi_i = \vec{n}_i \, \delta(\vec{r} - \vec{r}_{int})$, where $\vec{r}_{int}$ denotes a point on the interface between the two materials and $\vec{n}_i$ is the unit normal at this location pointing away from material i. That is, this term is nonzero only at the interface between the two materials and is an average of the micro-density over the subensemble of realizations for which $\vec{r}$ is an interface point. Clearly, it is related to the conditional pdf of the interface angular flux and cannot be expressed in terms of the interior pdf P_i in any obvious way. In fact this is just the familiar interface closure problem encountered in the previous approaches [3, 6] for which the Markov or LP-closure model was postulated in which the interface flux was simply replaced by the interior flux in an upwind sense. We recall that this closure is exact when the joint stochastic process of the angular flux and the material geometry is Markovian, specifically with Poisson material mixing statistics, i.e, for a purely absorbing material with exponentially distributed transition points and statistically independent sources. In the presence of scattering, the LP-closure is a model, and we adopt it here to close the interface term in Eq.(11). That is, we set

$$\langle \rho \frac{1}{\chi_i} \vec{\Omega} \cdot \nabla \chi_i \rangle \approx \frac{p_j \, P_j}{\lambda_j} - \frac{p_i \, P_i}{\lambda_i} \tag{13}$$

in Eq.(7) to obtain the following partially closed equation for the conditional pdf,

$$\begin{aligned} \frac{1}{v} \frac{\partial}{\partial t}(p_i \, P_i) \quad + \quad & \vec{\Omega} \cdot \nabla(p_i \, P_i) - S_i \frac{\partial}{\partial E}(p_i \, P_i) + \frac{\partial S_i}{\partial E} \frac{\partial}{\partial \psi}(\psi \, p_i \, P_i) - \sigma_{si} \frac{\partial}{\partial \psi}(\psi \, p_i \, P_i) = \\ & \frac{p_j \, P_j}{\lambda_j} - \frac{p_i \, P_i}{\lambda_i} - \frac{\partial}{\partial \psi} \int_{4\pi} d\vec{\Omega}' \int_0^\infty d\psi' \, \psi' \sigma_{si}(\vec{r}, E, \vec{\Omega} \cdot \vec{\Omega}') \, p_i \, P_{2i}(\psi, \psi'), \\ & \qquad i, j = 1, 2; \quad i \neq j, \end{aligned} \tag{14}$$

where we recall that λ_i, $i = 1, 2$ are the mean chord lengths for the two materials. Integrating Eq.(14) over all ψ and noting that the p_i are energy independent we obtain the following coupled set,

$$\frac{dp_i}{ds} = \frac{p_j}{\lambda_j} - \frac{p_i}{\lambda_i}, \quad i, j = 1, 2; \quad i \neq j, \tag{15}$$

which are just the Chapman-Kolmogorov equations for the material statistics with s measuring distance along a ray through the random medium. That is, the closure given by Eq.(13) correctly incorporates the material geometry in the limit of Poisson statistics. The Markov transition rates λ_i are implicitly functions of s, and hence of $\vec{r}$ and $\vec{\Omega}$, and are related to the p_i through Eq.(15). For homogeneous statistics, we note that $\frac{dp_i}{ds} = 0$ and Eq.(15) yields the simple result $p_i = \lambda_i / (\lambda_1 + \lambda_2)$, $i = 1, 2$. Since the λ_i can be interpreted as the mean chord lengths of each medium, we see that for homogeneous statistics the p_i are just the volume fractions of each material.

The equation for the conditional pdf, Eq.(14), is stochastically open because of the presence of the joint distribution in the scattering term. The simplest closure of this term is to neglect correlations between ψ and ψ', in which case the joint conditional pdf decomposes trivially into a product of the conditional marginal pdfs, i.e., $P_{2i}(\psi,\psi') \approx P_i(\psi)\,P_i(\psi')$. Eq.(14) then closes completely and reduces to the stochastic Liouville equation postulated in [3] under the assumption of a Markovian scattering source. This simple closure is equivalent, in the kinetic theory of gases, to the molecular chaos assumption used to truncate the BBGKY hierarchy at the lowest level, yielding the celebrated (nonlinear) Boltzmann equation. The correlation-neglect closure applied to Eq.(14) evidently also yields a nonlinear equation for the conditional pdf, but, as will become apparent in the next section, this is not the case. Clearly, higher order non-Markovian closures can be used in Eq.(14) for a more accurate representation of the scattering, but we defer such considerations to a future investigation. However, we make some additional remarks on this in the concluding section of this paper.

2.1. Moment Equations

In this section we consider equations for the conditionally averaged moments of the angular flux, which are defined by the following projection of the conditional pdf,

$$\psi_i^{(n)}(\vec{r},E,\vec{\Omega},t) = \int_0^\infty d\psi\,\psi^n\,P_i(\psi;\vec{r},E,\vec{\Omega},t), \quad i=1,2; \quad n=1,2\cdots \tag{16}$$

where, in particular, $\psi_i^{(1)} \equiv \psi_i$ is the familiar conditional mean angular flux [3]. Taking the first ψ-moment of Eq.(14), it can be shown that the conditional mean satisfies the following coupled transport equations,

$$\begin{aligned}\frac{1}{v}\frac{\partial}{\partial t}(p_i\,\psi_i) + \vec{\Omega}\cdot\nabla(p_i\,\psi_i) - \frac{\partial}{\partial E}(S_i\,p_i\,\psi_i) + \sigma_{si}\,p_i\,\psi_i &= \int_{4\pi} d\vec{\Omega}'\,\sigma_{si}(\vec{r},E,\vec{\Omega}\cdot\vec{\Omega}')\,p_i\,\psi_i(\vec{r},E,\vec{\Omega}',t) \\ &+ \frac{p_j\,\psi_j}{\lambda_j} - \frac{p_i\,\psi_i}{\lambda_i}, \quad i=1,2.\end{aligned} \tag{17}$$

In keeping with tradition, we refer to these equations as the standard model for electron transport in binary statistical media. What is striking about this result is that the scattering term is *exactly* closed at the level of the first ψ-moment. Unlike the equation for the conditional pdf, Eq.(14), the equations for ψ_1 and ψ_2 are entirely self-contained after the LP-closure has been applied to the interface terms. Thus, contrary to earlier derivations using stochastic approaches [3, 5], it is in fact not necessary to *a priori* approximate the scattering source as an independent source, uncorrelated with the angular flux. That is, with scattering described correctly, the stochastic Liouville or pdf approach is entirely consistent, at the level of the mean, with the direct conditional averaging method of Ref. [6]. From this observation one might conclude that the angular fluxes along different directions are uncorrelated, but this is only superficially so because correlations are extant in the equations for the higher order moments. In other words, the closure problem resurfaces for moments higher than the first. To see this explicitly, we take the general order ψ-moments of Eq.(11) and readily obtain,

$$\begin{aligned}&\frac{1}{v}\frac{\partial}{\partial t}(p_i\,\psi_i^{(n)}) + \vec{\Omega}\cdot\nabla(p_i\,\psi_i^{(n)}) - S_i\frac{\partial}{\partial E}(p_i\,\psi_i^{(n)}) - n\,\frac{\partial S_i}{\partial E}\,p_i\,\psi_i^{(n)} + n\,\sigma_{si}\,p_i\,\psi_i^{(n)} = \\ &n\int_{4\pi} d\vec{\Omega}'\int_0^\infty d\psi\int_0^\infty d\psi'\,\psi^{n-1}\,\psi'\sigma_{si}(\vec{r},E,\vec{\Omega}\cdot\vec{\Omega}')\,p_i\,P_{2i}(\psi,\psi') + \frac{p_j\,\psi_j^{(n)}}{\lambda_j} - \frac{p_i\,\psi_i^{(n)}}{\lambda_i}, \\ &\qquad i=1,2, \quad n=2,3\cdots\end{aligned} \tag{18}$$

The scattering integral contains the higher order expectation $\langle\psi^{n-1}\,\psi'\rangle$ and this indicates in particular that the conditional variance of the angular flux, defined by $V_i = \psi_i^{(2)} - \psi_i^2$, cannot be obtained exactly, even with the LP-closure for the interface terms. Closure models, synthetic or otherwise, must be developed to approximate these higher order correlations. The correlation-neglect closure, for instance, yields $\langle \psi^{n-1}\, \psi' \rangle \approx \langle \psi^{n-1} \rangle \, \langle \psi' \rangle$, and all moments can then be obtained successively using Eq.(18). Such a closure is robust and would provide estimates of the variance and higher order statistics which are at least consistent with the Markovian interface closure. Finally, we note that upon setting $P_{2i}(\psi, \psi') \approx P_i(\psi)\, P_i(\psi')$ in the scattering term in Eq.(14), the integral over ψ' can be effected to give the conditional mean angular flux $\psi_i(\vec{\Omega}')$. Moreover, since the equations for ψ_i were shown above to be self-contained, that is, independent of P_i, it follows that the equation for the conditional pdf is in fact linear when the correlation-neglect closure is used. Thus, the determination of the conditional mean angular fluxes completely determines all higher order one-point moments, indeed the entire one-point conditional pdf, in this approximation.

2.2. Mean Electron Energy Deposition

We now consider the application of our model to the computation of mean dose due to a time independent pencil beam of electrons incident on a binary statistical media. At this preliminary stage of our numerical investigations, we focus on the unconditional mean dose profile, which is defined by

$$D(\vec{r}) = \int_{4\pi} d\vec{\Omega} \int_0^{E_{max}} dE \, \left[p_1 S_1(E) \psi_1(\vec{r}, E, \vec{\Omega}) + p_2 S_2(E) \psi_2(\vec{r}, E, \vec{\Omega}) \right] \tag{19}$$

In particular we consider a binary mixture of alternating slabs with homogeneous Poisson mixing statistics, characterized by the one-point probabilities p_i and the rate parameters λ_i, which give the volume fraction and mean thickness or chord length of each material, respectively. The standard model given by Eq.(17) is solved in steady state one dimensional slab geometry using Monte Carlo simulation. Material transitions are readily handled by introducing pseudo-collisions, with cross section λ_i^{-1} describing the probability of an electron in material type i transitioning to one of type j. This interpretation is facilitated by noting that (ignoring CSD) Eq.(17) is analagous to a two group model with full coupling between groups and with the group transition constants given by λ_i^{-1}. The unconditional mean energy deposition is scored using the stopping power of each material, as defined in Eq.(19).

To test the accuracy of the standard model for high energy electron transport applications, benchmark results were also generated by analog Monte Carlo simulation of Eq.(1) for 10^4 realizations of the material geometry, and the unconditional mean dose and variance computed as a function of position. At selected spatial locations, we have also computed the unconditional pdf of the dose. We have not computed the dose variance for the standard model as yet since this requires consideration of flux correlations at different energies. This is a higher order statistical quantity that is not simply related to the variance in the angular flux for which a standard model was developed above. While our pdf method can be extended to formulate equations for correlations, numerical calculations are not straightforward and we defer such considerations to a later time. We will further comment on this briefly in the concluding section of this paper.

3. NUMERICAL RESULTS

Calculations presented here, that include elastic scattering and CSD energy loss, for both the standard model and the numerical benchmarks, were performed using a recently developed computationally efficient Monte Carlo technique for high energy electron transport based on a discrete scattering angle formalism [12]. The method has been extensively benchmarked against analog Monte Carlo simulations and demonstrated to give very accurate dose profiles using two discrete angles. Moreover, unlike condensed history methods and important for the present application, our approach is free of material interface artifacts [12]. Clearly, there are two sources of statistical uncertainties in our benchmark numerical results, one due to the finite number of material realizations and the other due to the finite number of particle histories. The only statistical error in the standard model simulations is that due to a finite number of histories. In both cases, enough samples (material and/or particles) were simulated to make the statistical uncertainties (in the mean dose and standard deviation) small enough and are not shown in the figures below. Where error bars are shown, they represent one standard deviation in the results due to the material randomness. Numerical benchmark results are labeled as "Benchmark" in the figures and results for the standard model are labeled as "Closure".

We consider first the non-scattering case, with a 1 MeV electron beam incident on a random mixture of gold and air, losing energy by continuous slowing down. The mean slab thicknesses λ_i were set to the respective electron mean free paths at the initial energy (in the 2 angle representation of the cross sections), in this case $\lambda_{Au} = 3 \times 10^{-4}$ cm and $\lambda_{air} = 2 \times 10^{3}$ cm. This corresponds to a very dilute concentration of a high energy deposition rate material (Au) in a predominantly low energy deposition rate material (air). The resulting unconditional mean dose profiles obtained from the standard model and the atomic mix limit are compared in Fig. 1 against the benchmark profile. As expected, the standard model predicts the dose

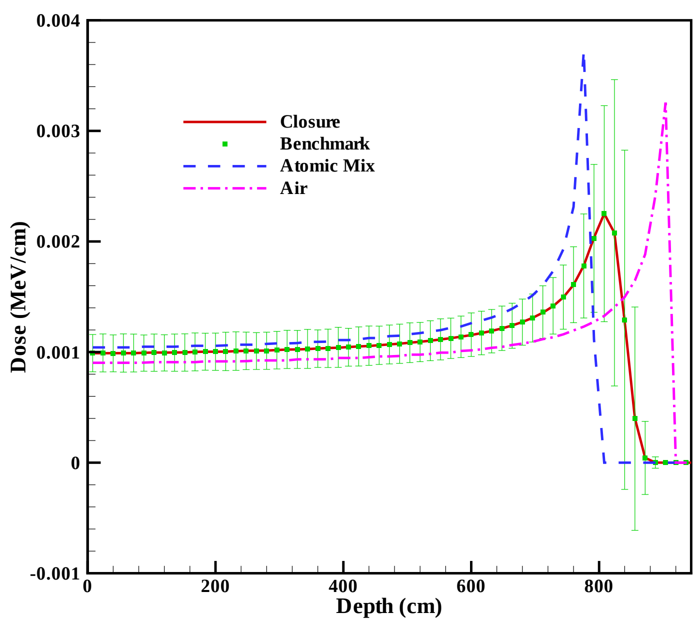

Figure 1. Pure CSD dose from 1 MeV electrons in gold-air mixture.

exactly when scattering is absent. That is, with all particles moving in the original forward direction while losing energy, the transport-material statistics are jointly Markovian for which the LP-closure provides an exact description. In contrast, the atomic mix result is considerably more peaked in magnitude and shallower in depth, consistent with the idealized Bragg distribution expected in a homogeneous non-scattering medium. For comparison and completeness, we have also shown the dose when the medium consists of air only and hence is inherently nonstochastic. The effect of a small amount of randomly mixed gold is starkly evident in this calculation, resulting in a highly straggled unconditional mean dose distribution in space when compared to the atomic mix result. Furthermore, the standard deviation in the dose is around 20%, which is clearly large for the relatively small volume fraction of gold.

The effects of scattering are shown in the dose profiles and pdfs in Fig. 2 through Fig. 5. For a

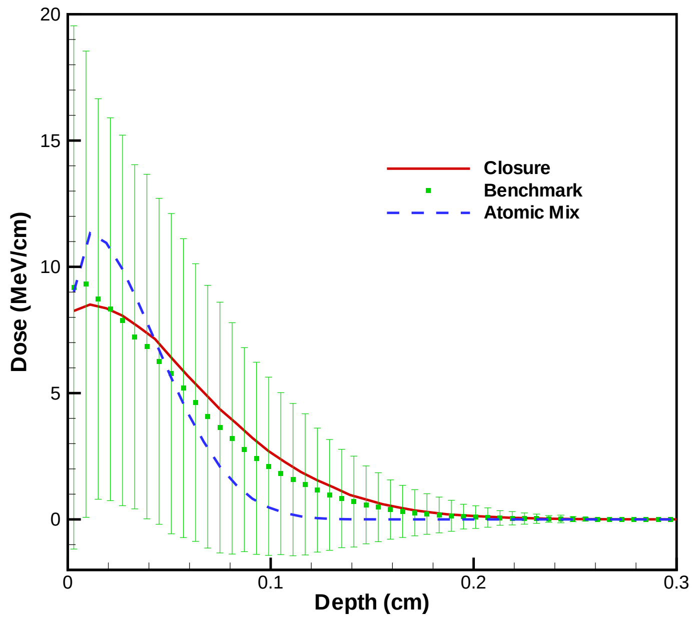

Figure 2. Dose from 1 MeV electrons in gold-silicon mixture

gold-silicon mixture, the dose profile is shown in Fig. 2 with mean slab thicknesses $\lambda_{Au} = 0.01$ cm and $\lambda_{Si} = 0.04$ cm, corresponding to a gold concentration of 20%. The standard model underpredicts the dose by about 12% near the surface and slightly overpredicts deeper into the medium, but it is significantly more accurate than atomic mix over all. In particular, it captures the straggled dose tail reasonably accurately. The corresponding dose pdf measured at approximately 0.06 cm is shown in Fig. 3. The structure of the dose pdf can be attributed to two variables: the amount of gold before reaching this layer and the amount of gold within the layer. For realizations with a lot of gold before the pdf layer, electrons will have little energy left to deposit when reaching the layer. Given that the mean thickness of the gold slabs is 0.01 cm, electrons will clearly see a reasonable amount of gold on average before the pdf layer is reached. This explains the broad peak at low doses in the pdf. For realizations with little gold before the pdf layer, electrons will in contrast reach the pdf layer with significant amounts of energy to deposit and the precise energy deposition rate will depend on the composition of the pdf layer.

For a water-air mixture, the dose profile for a 10 MeV incident electron beam is shown in Fig. 4 with mean slab thicknesses $\lambda_{H_2O} = \lambda_{air} = 0.5$ cm. The standard model is extremely accurate in this case indicating that the problem is near-Markovian. This is perhaps not surprising since this is an instance of highly forward peaked scattering, considerable more so than the gold-silicon case, so that the number of particles travelling in backward directions is likely to be very small. Hence the LP-closure is expected to be accurate in this case. We note, however, that the unconditional standard deviation is very large, indicating that the unconditional mean dose is not a reliable measure in this case. Given the disparate energy deposition characteristics of water and air, the observed statistical variability in the dose is not surprising. The

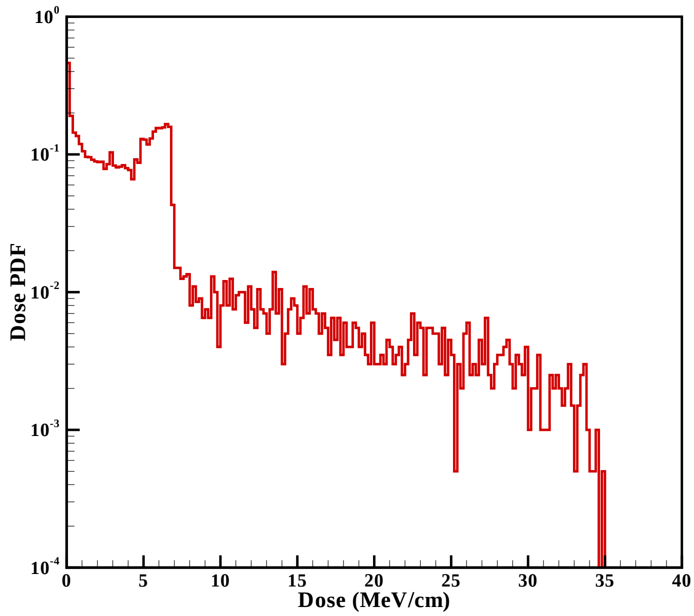

Figure 3. Dose PDF for gold-silicon mixture at a depth of 0.06 cm.

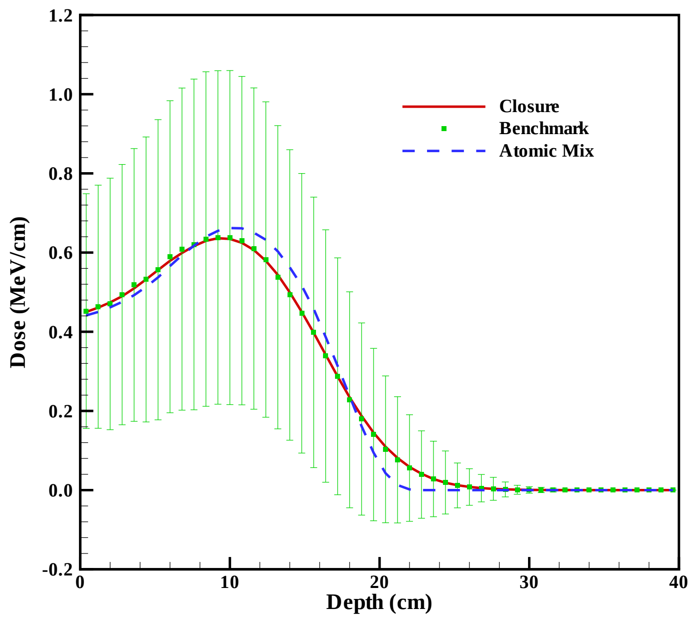

Figure 4. Dose from 10 MeV electrons in water-air mixture.

corresponding pdf at about 20 cm decreases monotonically (aside from statistical noise) with increasing dose with a long tail at large doses, and this highly non-Gaussian distribution illustrates why the one-sigma error bars in Fig. 4 extend below zero dose. Also, since the pdf layer is at a large depth compared to the

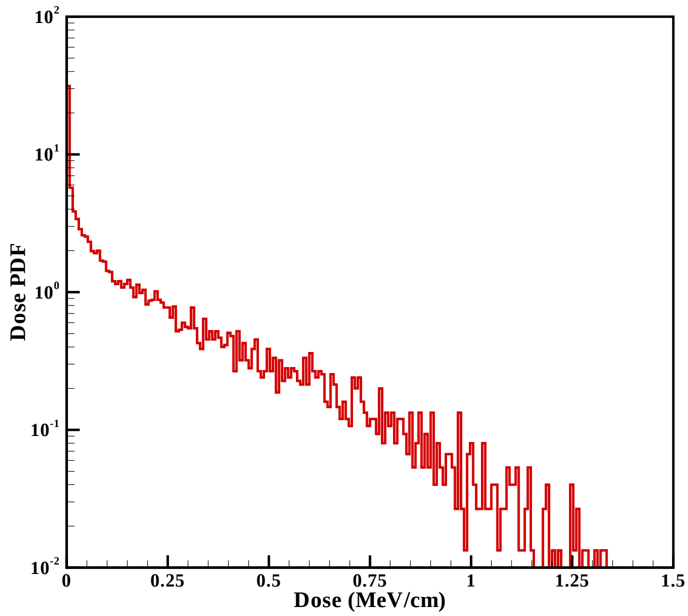

Figure 5. Dose PDF for water-air mixture at a depth of 20 cm.

mean slab thicknesses, there is a very low probability of having only one material before the pdf layer and this results in a much smoother dose pdf than in the gold-silicon mixture.

4. CONCLUSIONS AND FINAL REMARKS

The objective of this paper was twofold. First, to describe a consistent method for deriving equations for the conditional probability density of the angular flux in binary statistical media, that correctly incorporates *nonlocal* interactions such as scattering, and second, to apply this formalism to energy deposition or dose distribution calculations in such media due to high energy electrons. Two closure problems were demonstrated to arise in our kinetic theory based method: one was related to the random material transitions, for which the lowest order Levermore-Pomraning or Markovian closure model was used, and the other was the result of scattering induced correlations in the angular flux. However, the second closure problem was shown to vanish identically when equations for the conditional ensemble averaged flux were considered, although it resurfaced for all higher statistical averages.

Numerical results for the unconditional mean dose in binary gold-air and water-air mixtures were compared against benchmark results obtained for alternating slabs with Poisson statistics. The LP-closure model for the dose yields consistently more accurate results than the atomic mix limit for the cases considered. Also, the accuracy of the closure appears to increase as scattering becomes more forward peaked, consistent with the problem appearing increasingly jointly Markovian with decreasing numbers of backward moving particles.

The corresponding unconditional ensemble averaged standard deviation in the dose, computed from the benchmark simulations, was seen to be surprisingly large for these problems, while the unconditional dose pdfs, constructed at specific spatial locations also from the benchmark simulations, were observed to be highly nonsymmetric and non-Gaussian. One is led to conclude that lower order statistical averages, in particular the unconditional mean and standard deviation, are not sufficient to comprehensively characterize electron energy deposition in binary random media. However, it may be more meaningful to consider *conditional* averages when material physical properties are highly contrasting. This would be true in water-air (or tissue-air) mixtures, for instance, where one is typically not interested in the energy deposited in the air, while the conditional variance of the dose in the water is likely to be smaller than the unconditional variance reported here. These considerations will form the subject of future work.

Several generalizations of the work presented here can be envisioned and, indeed, may be deemed necessary in order to realize the full potential of the pdf approach. In concluding this paper we briefly mention a few important extensions. First, and perhaps most pressing, is that the inscattering term in Eq.(14), which describes correlations between the angular flux in different directions, must be closed. That is, the two-point joint pdf $P_{2i}(\psi, \psi'; \vec{\Omega}, \vec{\Omega}')$ must be expressed in terms of the marginal pdfs $P_i(\psi, \vec{\Omega})$ and $P_i(\psi', \vec{\Omega}')$. While an explcit equation for $P_{2i}(\psi, \psi'; \vec{\Omega}, \vec{\Omega}')$ may be derived using the techniques of this paper, the result will be a higher dimensional equation (having ψ' and $\vec{\Omega}'$ as additional independent variables) and, furthermore, it will also suffer from a closure problem through the appearance of a triple correlation term. A simpler approach is to construct synthetic closures that interpolate between certain known limiting or special cases. For instance, we are currently investigating a one parameter closure that linearly interpolates between the uncorrelated and fully correlated ($\vec{\Omega}' = \vec{\Omega}$) limits. The parameter can be regarded as free, chosen to give the best solution in some sense, or it can be determined empirically, from a knowledge of the correlation coefficient, for example.

Second, the one-point pdf of the angular flux that has been the focus of this paper cannot be used to determine the pdf, and hence the variance and higher statistical averages, of the dose. Since energy deposition in each realization is related to the integral over energy and direction of the angular flux (see Eq.(19)), the pdf of the dose will involve infinite order correlations in energy and angle of the angular flux and hence will be related to the joint distribution of the angular flux over *all* energies and directions, i.e., to the probability density *functional* of the angular flux. While an equation for the latter can be written down, it will be formal and impractical for computational purposes. In general, for quantities that are functionals of the angular flux, the forward master equation approach [11] that we have essentially adopted here is not suitable. However, a backward or adjoint approach may prove more fruitful and we are currently developing such a formalism.

Finally, the pdf approach may provide a systematic way of constructing a higher order closure of the material transition terms, which at lowest order would yield the Markovian or LP-closure. Recall that this closure problem is manifest through the appearance of averages over the subensemble of points that are located on material interfaces, giving rise to ensemble averaged interface angular fluxes as additional unknowns. One approach to dealing with this difficulty may be to focus on the joint pdf of the interior and interface fluxes, the motivation being that by suitably expanding the space of the pdf a jointly Markovian system can sometimes be achieved. A closed equation (aside from the scattering terms) for the higher dimensional pdf may then be derived and moment equations generated. There is no a priori indication whether or not such an approach would be successful, but we believe that the idea merits consideration.

ACKNOWLEDGEMENTS

The work of the first author was supported in part by the US Department of Energy under contract DE-FG07-02ID14336 with the University of New Mexico. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

REFERENCES

[1] G. C. Pomraning, *Transp. Theory Stat. Phys.*, **27**, 405 (1998).

[2] C. D. Levermore, G. C. Pomraning, D. L Sancho and J. Wong, *J. Math. Phys.*, **27**, 2526 (1986).

[3] G. C. Pomraning, *Linear Kinetic Theory and Particle Transport in Stochastic Mixtures*, World Scientific, Singapore (1991).

[4] D. Vanderhaegan, *J. Quant. Spectrosc. Radiat. Transfer*, **36**, 557 (1986).

[5] D. Vanderhaegan and C. Deutsch, *J. Statist. Phys*,**54**, 331 (1989).

[6] M. L. Adams, E. W. Larsen, and G. C. Pomraning, *J. Quant. Spectrosc. Radiat. Transfer*, **42**, 253 (1989).

[7] Yu L. Klimontovich, *Kinetic Theory of Nonideal Gases and Nonideal Plasmas*, Pergamon Press, New York (1982).

[8] M. M. R. Williams, *Mathematical Methods in Particle Transport Theory*, Butterworths, London (1971).

[9] S. Edwards, *J. Fluid Mech.*, **18**, 239 (1964).

[10] S. Pope, *Prog. Energy Combust. Sci.*, **11**, 119 (1985).

[11] N. G. Van Kampen, *Stochastic Processes in Physics and Chemistry*, North Holland, New York (1981).

[12] B. C. Franke and A. K. Prinja, “Monte Carlo Electron Dose Calculations Using Discrete Scattering Angles and Discrete Energy Losses,” *these Proceedings*.