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ESTIMATING ANISOTROPIC DIFFUSION OF NEUTRONS NEAR THE BOUNDARY OF A PEBBLE BED RANDOM SYSTEM

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ABSTRACT

Due to the arrangement of the pebbles in a Pebble Bed Reactor (PBR) core, if a neutron is located close to a boundary wall, its path length probability distribution function in directions of flight parallel to the wall is significantly different than in other directions. Hence, anisotopic diffusion of neutrons near the boundaries arises. We describe an analysis of neutron transport in a simplified 3-D pebble bed random system, in which we investigate the anisotropic diffusion of neutrons born near one of the system's boundary walls. While this simplified system does not model the actual physical process that takes place near the boundaries of a PBR core, the present work paves the road to a formulation that may enable more accurate diffusion simulations of such problems to be performed in the future. Monte Carlo codes have been developed for (i) deriving realizations of the 3-D random system, and (ii) performing 3-D neutron transport inside the heterogeneous model; numerical results are presented for three different choices of parameters. These numerical results are used to assess the accuracy of estimates for the mean-squared displacement of neutrons obtained with the diffusion approximations of the Atomic Mix Model and of the recently introduced [1] Non-Classical Theory with angular-dependent path length distribution. The Non-Classical Theory makes use of a Generalized Linear Boltzmann Equation in which the locations of the scattering centers in the system are correlated and the distance to collision is not exponentially distributed. We show that the results predicted using the Non-Classical Theory successfully model the anisotropic behavior of the neutrons in the random system, and more closely agree with experiment than the results predicted by the Atomic Mix Model.

Key Words: random media, pebble bed, anisotropic diffusion, Monte Carlo

1. INTRODUCTION

The Pebble Bed Reactor (PBR) is a graphite-moderated, gas-cooled, very high temperature reactor. It uses spherical fuel elements called pebbles, which are made of pyrolytic graphite (the moderator), containing thousands of microscopic fuel Tristructural-isotropic particles, each of which consists of a fissile material surrounded by a coated ceramic layer of SiC for structural integrity. Thousands of pebbles are placed together in the PBR core, which is cooled by an inert or semi-inert gas such as helium.

Inside the core, the pebbles are piled on top of one another in a "random" manner. Typically, the neutronic modeling of the geometrically random core is done by: (i) developing self-shielded multigroup cross sections for the pebbles, (ii) volume-averaging these cross sections over the entire core, including the helium-filled region between the pebbles (the *Atomic Mix Model*), and (iii) using the spatially-homogenized cross sections in a diffusion code.

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Step (ii) in the procedure described above leads to certain issues. First, the Atomic Mix approximation is known to be accurate only when the chunk sizes of the constituent materials are small compared to a mean free path. However, PBR pebbles are not optically thin; they are O(1) mean free paths thick. The second issue is that, due to geometrical effects, neutrons located close to the wall of the core tend to travel significantly larger distances between collisions in directions of flight parallel to the wall. Thus, neutron transport and diffusion are affected in an anisotropic manner that is not modeled by the Atomic Mix approximation.

Previous work has been carried out to investigate the diffusion of neutrons in the *center* of a model 3-D PBR core, away from the effects of the outer boundaries [1]. This past work has shown that, in the center of the PBR core, (i) anisotropic diffusion of neutrons caused by the gravitational piling of pebbles is nearly neglectable, and (ii) the Non-Classical Theory, when compared to Monte Carlo results, is significantly more accurate than the Atomic Mix Model in predicting the mean-squared displacement of neutrons.

Here, we extend this previous analysis in order to assess the accuracy of the Non-Classical Theory in predicting the anisotropic behavior of neutrons that are born near the boundaries of a 3-D pebble bed random system. To perform this assessment, we have developed (i) a Monte Carlo computer code to derive realizations of the random system, and (ii) a second Monte Carlo code that performs neutron transport inside this heterogeneous model. We use these codes to generate numerical results for important microscopic (mean and mean-squared free path) and macroscopic (mean-squared displacement) quantities. These numerical results are then compared to estimates for the mean-squared displacement of neutrons from their point of birth, obtained from the asymptotic diffusion approximation of two different models: the Atomic Mix Model and the Non-Classical Theory.

We remark that, due to non-physical characteristics of the simplified model (discussed in Section 3), the numerical results obtained in this paper do not reflect the actual physical process encountered near the boundaries of a PBR core. Nevertheless, these results allow us to validate the accuracy of the Non-Classical Theory predictions of anisotropic diffusion, and are therefore employed for that purpose.

In Section 2 of this paper, we sketch the formulations for the Atomic Mix Model and the Non-Classical Theory, including their asymptotic diffusion approximations. In Section 3 we describe the Monte Carlo codes used to create the random realizations of the model and to simulate neutron transport in these heterogeneous media. We then present numerical results for three different choices of parameters, and show that the estimates for mean-squared displacement obtained with the Non-Classical Theory successfully model the anisotropy of the diffusion and are more accurate than the ones obtained with the Atomic Mix Model. We conclude with a brief discussion of our results and an outline of future steps in Section 4.

2. ATOMIC MIX MODEL AND NON-CLASSICAL THEORY FORMULATIONS

We consider a binary random system composed of *chunks* of material 1 embedded in a background material 2. In this case, we define $\Sigma_{t,i}$ and c_i respectively as the total cross section and scattering ratio of material i, for $i \in \{1, 2\}$. 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 defining the path length traveled by the neutron since its previous interaction (birth or scattering) as s, we make the following assumptions: **(i)** the physical system is statistically homogeneous and has azimuthal symmetry; **(ii)** neutron transport is monoenergetic; **(iii)** neutron transport is driven by a specified point source located at the origin and isotropically emitting Q neutrons per second; **(iv)** the neutron flux $\rightarrow 0$ as $|\boldsymbol{x}| \rightarrow \infty$; **(v)** scattering is isotropic.

Given a single realization of this random system, we can write the packing fraction of material 1 as

$$\Gamma = \frac{\text{total volume occupied by material 1 in the system}}{\text{total volume of system}}. \tag{1}$$

Then, ensemble-averaging over all possible realizations of the system, the Atomic Mix parameters are given by

$$\big\langle \Sigma_t \big\rangle = \text{volume-averaged total cross section} = \big\langle \Gamma \big\rangle \Sigma_{t,1} + \big(1 - \big\langle \Gamma \big\rangle\big)\Sigma_{t,2}; \tag{2a}$$

$$\big\langle c\Sigma_t \big\rangle = \text{volume-averaged scattering cross section} = \big\langle \Gamma \big\rangle c_1\Sigma_{t,1} + \big(1 - \big\langle \Gamma \big\rangle\big)c_2\Sigma_{t,2}. \tag{2b}$$

The steady-state Atomic Mix equation [2] for this system [with an isotropic point source at $(x, y, z) = (0, 0, 0)$] is:

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \big\langle \psi(\boldsymbol{x}, \boldsymbol{\Omega}) \big\rangle + \big\langle \Sigma_t \big\rangle \big\langle \psi(\boldsymbol{x}, \boldsymbol{\Omega}) \big\rangle = \frac{\big\langle c\Sigma_t \big\rangle}{4\pi} \big\langle \Phi(\boldsymbol{x}) \big\rangle + \frac{Q}{4\pi}\delta(x)\delta(y)\delta(z), \tag{3}$$

where $\big\langle \Phi(\boldsymbol{x}) \big\rangle = \int_{4\pi} \big\langle \psi(\boldsymbol{x}, \boldsymbol{\Omega}) \big\rangle d\Omega$. Defining $\big\langle \Sigma_a \big\rangle = \big\langle \Sigma_t \big\rangle - \big\langle c\Sigma_t \big\rangle$, the asymptotic diffusion approximation for the Atomic Mix Eq. (3) is

$$-\mathrm{D}\,\nabla^2 \big\langle \Phi(\boldsymbol{x}) \big\rangle + \big\langle \Sigma_a \big\rangle \big\langle \Phi(\boldsymbol{x}) \big\rangle = Q\delta(x)\delta(y)\delta(z), \tag{4a}$$

$$\mathrm{D} = \frac{1}{3\big\langle \Sigma_t \big\rangle}. \tag{4b}$$

Similarly to classical transport in a homogeneous medium, the Atomic Mix Model assumes that the ensemble-averaged probability distribution function $p(\boldsymbol{\Omega}, s)$ [of the random distances s traveled between collisions in the direction $\boldsymbol{\Omega}$] is exponential and independent of $\boldsymbol{\Omega}$: $p(\boldsymbol{\Omega}, s) = p(s) = \big\langle \Sigma_t \big\rangle e^{-\langle \Sigma_t \rangle s}$. In this case, $\big\langle s \big\rangle = 1/\big\langle \Sigma_t \big\rangle$ and $\big\langle s^2 \big\rangle = 2\big\langle s \big\rangle^2$.

However, for the problem we want to approach, the geometrical arrangement of the pebbles will cause $p(\boldsymbol{\Omega}, s)$ to be non-exponential. Specifically, in a random system such as the PBR core, while the *optical* distance to collision in each realization of the system can be calculated from an exponential, the ensemble-averaged probability distribution function for the *non-optical* random distance to collision s in the direction $\boldsymbol{\Omega}$ will generally be a non-exponential function of s and $\boldsymbol{\Omega}$.

One can obtain a formulation of $p(\boldsymbol{\Omega}, s)$ as follows. For a specific realization of the core, let $\boldsymbol{x}$ be a random point inside one of the pebbles, and $\boldsymbol{\Omega}$ a random direction of flight. Then, if

$$P(\boldsymbol{x}, \boldsymbol{\Omega}, s) = \Sigma_t(\boldsymbol{x} + s\boldsymbol{\Omega}) e^{-\int_0^s \Sigma_t(\boldsymbol{x} + s'\boldsymbol{\Omega}) ds'}, \tag{5}$$

the probability that a neutron released at $\boldsymbol{x}$ in the direction $\boldsymbol{\Omega}$ will experience its first collision while traveling a distance between s and $s + ds$ is given by $P(\boldsymbol{x}, \boldsymbol{\Omega}, s)ds$. Thus, for this realization, $P(\boldsymbol{x}, \boldsymbol{\Omega}, s)$ is the distribution function for the distance to collision s for a particle released at $\boldsymbol{x}$ in the direction $\boldsymbol{\Omega}$. Then $p(\boldsymbol{\Omega}, s)$ is the ensemble average of $P(\boldsymbol{x}, \boldsymbol{\Omega}, s)$ over all scattering centers $\boldsymbol{x}$ in the realization, and over all possible realizations. Finally, it can be shown that [1]

$$\Sigma_t(\boldsymbol{\Omega}, s) = \frac{p(\boldsymbol{\Omega}, s)}{1 - \int_0^s p(\boldsymbol{\Omega}, s') ds'}. \tag{6}$$

We now add to our assumptions that **(vi)** $\Sigma_t(\boldsymbol{\Omega}, s)$ is known. Keeping in mind the other assumptions already made, we can use the Non-Classical Theory [3–5] to write the Generalized Linear Boltzmann Equation with

angular dependent path length distribution [1] for this system:

$$\frac{\partial\psi}{\partial s}(\boldsymbol{x},\boldsymbol{\Omega},s)+\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},s)+\Sigma_t(\boldsymbol{\Omega},s)\psi(\boldsymbol{x},\boldsymbol{\Omega},s) = \frac{\delta(s)}{4\pi}c\int_{4\pi}\int_0^\infty \Sigma_t(\boldsymbol{\Omega}',s')\psi(\boldsymbol{x},\boldsymbol{\Omega}',s')ds'd\Omega'+\delta(s)\frac{Q}{4\pi}\delta(x)\delta(y)\delta(z). \tag{7}$$

Defining $\left\langle s^2_{\boldsymbol{\Omega}}\right\rangle(\boldsymbol{\Omega})$ as the mean-squared free path of a neutron in the direction $\boldsymbol{\Omega}$, we can write the asymptotic diffusion approximation for Eq. (7) as

$$-\mathrm{D}_x\frac{\partial^2}{\partial x^2}\Phi(\boldsymbol{x})-\mathrm{D}_y\frac{\partial^2}{\partial y^2}\Phi(\boldsymbol{x})-\mathrm{D}_z\frac{\partial^2}{\partial z^2}\Phi(\boldsymbol{x})+\frac{1-c}{\left\langle s\right\rangle}\Phi(\boldsymbol{x})=Q\delta(x)\delta(y)\delta(z), \tag{8a}$$

$$\mathrm{D}_u=\frac{1}{2\left\langle s\right\rangle}\frac{1}{4\pi}\int_{4\pi}\left\langle s^2_{\boldsymbol{\Omega}}\right\rangle(\boldsymbol{\Omega})\Omega_u^2 d\Omega. \tag{8b}$$

From Eq. (8b), the diffusion coefficients given by the Non-Classical Theory can differ in different directions. We will show that this feature allows this theory to model the diffusion in this problem more accurately than the Atomic Mix Model.

Finally, recalling that $\Phi(\boldsymbol{x})\rightarrow 0$ and $\nabla\Phi(\boldsymbol{x})\rightarrow 0$ as $|\boldsymbol{x}|\rightarrow\infty$, we can manipulate Eqs. (4a) and (8a) to derive an exact (diffusion) formula for the mean-squared displacement of neutrons. To do this, we multiply these equations by $x^2+y^2+z^2$ and integrate over $-\infty<x,y,z<\infty$. Noting that for $u=x,y,z$

$$\int_{-\infty}^{\infty}u^2\frac{\partial^2\Phi}{\partial u^2}du=-2\int_{-\infty}^{\infty}u\frac{\partial\Phi}{\partial u}du=2\int_{-\infty}^{\infty}\Phi du, \tag{9}$$

we obtain the result

$$\left\langle u^2\right\rangle=\frac{\int_{-\infty}^{\infty}u^2\Phi(\boldsymbol{x})du}{\int_{-\infty}^{\infty}\Phi(\boldsymbol{x})du}=2\frac{\mathrm{D}_u}{Absorption}, \tag{10a}$$

$$\left\langle \rho^2\right\rangle=\frac{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(x^2+y^2+z^2)\Phi(\boldsymbol{x})dxdydz}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Phi(\boldsymbol{x})dxdydz}=2\frac{\left(\mathrm{D}_x+\mathrm{D}_y+\mathrm{D}_z\right)}{Absorption}, \tag{10b}$$

where $Absorption=\left\langle\Sigma_a\right\rangle$ for the Atomic Mix Model and $Absorption=(1-c)/\left\langle s\right\rangle$ for the Non-Classical Theory.

3. NUMERICAL RESULTS AND MODEL ESTIMATES

We consider a random system that models a simplified PBR core. Specifically, we make the following assumptions:

- Each pebble is modeled as a homogeneous sphere of radius r.
- Using the ballistic deposition algorithm described in Section 3.1, pebbles are randomly placed in a cubic box with sides of length L.
- Neutron transport occurs in a "quasi-periodic" semi-infinite system, with one outer boundary wall perpendicular to the x-axis. This system is constructed by extending the pebble arrangement in the cubic box as described in Section 3.2.

- Neutrons are monoenergetic and scatter isotropically.
- Neutrons are born inside pebbles that touch the boundary wall of the system.
- The boundary wall is reflective.

At this point, it is important to remark that the choice of a reflective boundary is *not* physically correct. While in reality a portion of the neutrons that escape will not return to the core, most escaped neutrons will (ideally) reenter the system at some other point after traveling in the outer shell that envelops the core. This effect is clearly not captured with the choice of a reflective boundary condition, and as a result the quantities presented in this work do not reflect the actual physical problem.

However, the choice of a reflective boundary condition (i) greatly simplifies the computational aspects of the work; and (ii) allows us to mathematically model the problem as an infinite system (with a "mirror image" at the boundary wall). While in the future we hope to apply the Non-Classical Theory in physically accurate models, the main goal of this paper is to assess the accuracy of the Non-Classical Theory and its improvement over the Atomic Mix approach in predicting anisotropic diffusion of neutrons in certain regions of a pebble bed random system.

We have written a Monte Carlo computer code that constructs random realizations of the simplified model core, and a second Monte Carlo code that performs neutron transport inside the heterogeneous core. In this manner, we have simulated neutron transport in the random realizations of the core and compared the numerical results to estimates obtained from the Atomic Mix and the Non-Classical Theory models. In the remainder of this section, we give details of these algorithms and the subsequent results.

3.1. Random Packing of pebbles in the Model Core

To obtain the 3-D random packings studied in this work, we adapted the algorithm proposed in [1], which consists of a variation of the ballistic deposition method [6]. In our "ballistic" algorithm, each spherical pebble is released at a random point above the box. It then follows a steepest descent trajectory until it reaches a position that is stable under gravity, in which case its coordinates are stored.

To construct a realization of the system, we randomly drop and store the coordinates of 20 different *tentative* pebbles; we then choose the one with the lowest z-coordinate to be added to the system, and discard the 19 remaining ones. Once a pebble is added to the system, its position is locked; that is, the pebble is frozen in place.

Rearrangement of pebbles and/or cascading events cannot happen. No velocity or friction coefficients are taken into account; the only restriction is that a pebble can never, at any point of its trajectory, overlap the limits of the box or another pebble. Once the tentative pebble with the lowest z-coordinate is added to the system, the process is repeated; pebbles continue to be added until the box is filled. An example of a random piling obtained with this procedure is shown in Figure 1.

We have developed 50 different random packings in a 3-D system with $L = 100r$. Defining the pebbles as material 1, the packing fraction of pebbles in a single realization of the system is given by Eq. (1), and we found the average packing fraction to be $\langle \Gamma \rangle = 0.5791$, with a standard deviation of 0.0009.

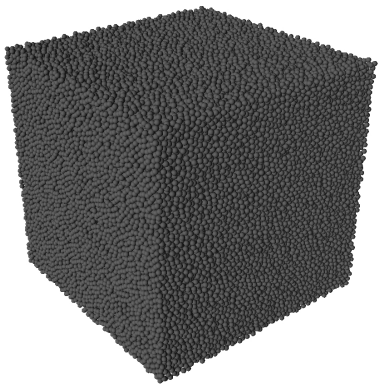

Figure 1. Example of a 3-D Random Piling in a Box with Side $L = 100r$

3.2. Monte Carlo Transport in the Model Core

Each realization of the problem is composed of solid spheres (pebbles of material 1) immersed in a void background (material 2). If we consider a neutron that is born (or scatters) at a random point (x, y, z) inside a specific pebble, the total *optical distance* that this neutron will travel before experiencing a collision (that is, the distance it travels *inside the pebbles*) is sampled from the exponential distribution $p(s) = \Sigma_{t,1} e^{-\Sigma_{t,1} s}$.

For all realizations described in this work, the packing of pebbles of radius r took place in a cubic box with side $L = 100r$. This box of side L was assumed to have its center at the origin; that is, the coordinates of the system satisfy $-L/2 \leq x, y, z \leq L/2$. We are interested in investigating the histories of neutrons that are born close to the wall positioned at the plane $x = -L/2$.

To minimize the effect of the other five boundaries of the box, the system in which neutrons are allowed to travel does not contain all the pebbles in the packing. According to the work in [7], one needs to consider pebbles that are three to five diameters away from a specific boundary in order to have a packing structure that is not influenced by it. In our simulations we found that, for each different realization of the system, the fluctuations in the local packing fractions ceased being significant around two diameters away from each wall of the box (≈ 0.594), as was the case in the experiment performed by Lieberoth & Stojadinović [8].

Thus, for the sake of accuracy, we do not allow neutrons to travel within a distance of three diameters to the five walls of the box located at $x = L/2$, $y = \pm L/2$, and $z = \pm L/2$. If a neutron travels within any of these regions, the system is shifted so that the neutron is "reinserted" back in the interior of the box, away from the boundaries. This "reinsertion" process, introduced and described in detail in [1], can be interpreted as meaning that neutrons are traveling in a semi-infinite (with a boundary at $x = -L/2$) "quasi-periodic" structure. The term "quasi-periodic" used here means that the coordinates of the system do not always shift by the same values in a given direction.

Given a realization of the model core, we select a pebble that rests against the wall at $x = -L/2$ to be the one in which neutrons are born (i.e., we focus on the transport of neutrons generated by a single fuel pebble). The neutrons subsequent histories within the system are determined by our Monte Carlo transport code, which numerically calculates:

- $\left\langle s_{\mathbf{\Omega}} \right\rangle (\mathbf{\Omega})$ = mean distance to collision (mean free path) in the direction $\mathbf{\Omega}$;

- $\langle s \rangle$ = mean distance to collision (mean free path);
- $\langle s^2_{\mathbf{\Omega}} \rangle(\mathbf{\Omega})$ = mean-squared distance to collision (mean-squared free path) in the direction $\mathbf{\Omega}$;
- $\langle s^2 \rangle$ = mean-squared distance to collision (mean-squared free path);
- $\langle x^2 \rangle$, $\langle y^2 \rangle$, $\langle z^2 \rangle$ = mean-squared displacement of a neutron in the directions x, y, and z, respectively;
- $\langle \rho^2 \rangle = \langle x^2 + y^2 + z^2 \rangle$ = mean-squared displacement of a neutron.

Since the background material 2 is assumed to be vacuum, $\Sigma_{t,2} = \Sigma_{s,2} = \Sigma_{a,2} = 0$. We selected three different sets of cross sections for material 1 (pebbles). The fuel pebbles were chosen in each realization to be centered at a distance of $\varepsilon = r$ of the system's boundary at $x = -L/2$ (that is, touching the wall). It has been shown that the anisotropic effect in the z-direction of such model cores due to the gravitational piling of pebbles is very small [1]. Therefore, if we consider pebbles located away from the y and z boundaries of the box, a realization containing N pebbles with coordinates (x_n, y_n, z_n) and a realization containing N pebbles with coordinates (x_n, z_n, y_n), where $1 \leq n \leq N$, have nearly the same probability of occurring. Thus, if we measure the polar angle with respect to the x-axis, the resulting ensemble-averaged system (over all possible realizations) will have azimuthal symmetry. In other words, $\langle y \rangle = \langle z \rangle$ and $\langle y^2 \rangle = \langle z^2 \rangle$ in the ensemble-averaged system. The parameters of the pebbles in each problem are presented in Table I.

Table I. Parameters of the pebbles in the Simulations

Problem	$2r\Sigma_{t,1}$	$2r\Sigma_{s,1}$	$2r\Sigma_{a,1}$	$c_1 = \Sigma_{s,1}/\Sigma_{t,1}$	$P(\mathbf{\Omega} \cdot \mathbf{\Omega})$
1	1.0	0.99	0.01	0.99	1/4π
2	2.0	1.995	0.005	0.9975	1/4π
3	4.0	3.9975	0.0025	0.999375	1/4π

Table II. Ensemble-Averaged Monte Carlo Transport Results

Problem	$\langle s \rangle / 2r$	$\langle s^2 \rangle / 4r^2$	$\langle x^2 \rangle / 4r^2$	$\langle y^2 \rangle / 4r^2$	$\langle \rho^2 \rangle / 4r^2$
1	1.7271	6.4795	210.8987	216.7292	644.3571
2	0.8634	1.7611	225.9157	232.6521	691.2200
3	0.4316	0.5184	255.8249	264.6351	785.0952

For each of the 50 realizations of the random system, we calculated the histories of 1,000,000 neutrons (summing to a total of 50,000,000 neutrons' histories); the statistical error in each realization was found to

be (with 97.5% confidence) less than 0.057% for all collected data values. The ensemble-averaged Monte Carlo results are given in Table II, and the statistical error bounds (with 95% confidence) are presented in Table III.

Table III. Relative Statistical Errors (%) of Ensemble-Averaged Monte Carlo Transport Results

Problem	$\langle s \rangle / 2r$	$\langle s^2 \rangle / 4r^2$	$\langle x^2 \rangle / 4r^2$	$\langle y^2 \rangle / 4r^2$	$\langle \rho^2 \rangle / 4r^2$
1	0.1299	0.2848	0.2908	0.2614	0.2327
2	0.1130	0.2748	0.2549	0.2711	0.2398
3	0.0971	0.2757	0.2262	0.2260	0.2021

We can clearly observe the expected anisotropic effect: the mean-squared displacement of neutrons in the directions parallel to the wall (y and z) is $\approx 3\%$ larger than in the x-direction, increasing from a difference of 2.8% in Problem 1 to 3.4% in Problem 3.

3.3. Atomic Mix Model and Non-Classical Theory Estimates

To obtain estimates for the mean-squared displacement of neutrons from their point of birth, we must combine Eqs. (10) with the appropriate expressions for Σ_a and D_u. In the present case, we obtain

$$\left\langle u^2 \right\rangle = \begin{cases} \frac{1}{2(1-c_1)} \frac{1}{4\pi} \int_{4\pi} \left\langle s^2_{\mathbf{\Omega}} \right\rangle (\mathbf{\Omega}) \Omega_u^2 d\Omega & \text{Non-Classical Theory} \\ \\ \frac{2}{3} \frac{1}{\left\langle \Gamma \right\rangle^2 \Sigma_{t,1} \Sigma_{a,1}} & \text{Atomic Mix Model} \end{cases} . \tag{11}$$

Not surprisingly, the Non-Classical Theory and the Atomic Mix Model predict different mean-squared displacements of neutrons. In particular, the Atomic Mix predictions depend strongly on the choice of the average packing fraction $\left\langle \Gamma \right\rangle$. The underlining question is: what value should be chosen for the average packing fraction? There is a sharp transition in the packing fraction as one moves away from the wall: the average packing fraction varies from 0 (exactly at the wall) to 0.4698 (within one diameter away from the wall) and then to 0.5936 (over three diameters away from the wall, in the interior of the system).

We investigate the results obtained for three different choices of $\left\langle \Gamma \right\rangle$, namely: $\left\langle \Gamma_1 \right\rangle = 0.4698$ (the average packing fraction within distances of $2r$ from the wall); $\left\langle \Gamma_2 \right\rangle = 0.5482$ (the average packing fraction within distances of $6r$ from the wall); and $\left\langle \Gamma_3 \right\rangle = 0.5791$ (the average packing fraction of the full cubic system).

Using (i) Eqs. (10) and (11), (ii) Table I for $\Sigma_{t,1}$, $\Sigma_{a,1}$, and c_1, and (iii) the numerically obtained values of $\left\langle s^2_{\mathbf{\Omega}} \right\rangle (\mathbf{\Omega})$, we obtain the estimates of the root mean-squared displacement of neutrons from their point of birth shown in Table IV. Here, the Monte Carlo error is estimated using the Central Limit Theorem with 95.0% confidence, and the Non-Classical Theory and Atomic Mix Model errors are the percent relative differences between their estimates and the Monte Carlo estimate for the root mean-squared displacement.

Table IV. Estimates of the root mean-squared displacement of neutrons from their Point of Birth

Problem	Model	$\frac{\langle x^2 \rangle^{1/2}}{2r}$	Error(%)	$\frac{\langle y^2 \rangle^{1/2}}{2r}$	Error(%)	$\frac{\langle \rho^2 \rangle^{1/2}}{2r}$	Error(%)
.	Monte Carlo	14.5224	0.1454	14.7217	0.1307	25.3842	0.1164
.	Non-Classical	14.6439	0.8372	14.7225	0.0052	25.4548	0.2781
1	Atomic Mix (Γ_1)	17.3804	19.6806	17.3804	18.0598	30.1038	18.5927
.	Atomic Mix (Γ_2)	14.8939	2.5586	14.8939	1.1697	25.7970	1.6264
.	Atomic Mix (Γ_3)	14.0990	2.9154	14.0990	4.2302	24.4201	3.7979
.	Monte Carlo	15.0305	0.1275	15.2529	0.1355	26.2911	0.1199
.	Non-Classical	15.2756	1.6309	15.3474	0.6193	26.5411	0.9510
2	Atomic Mix (Γ_1)	17.3804	15.6345	17.3804	13.9481	30.1038	14.5213
.	Atomic Mix (Γ_2)	14.8939	0.9086	14.8939	2.3537	25.7970	1.8656
.	Atomic Mix (Γ_3)	14.0990	6.1976	14.0990	7.5656	24.4201	7.1134
.	Monte Carlo	15.9945	0.1131	16.2676	0.1130	28.0195	0.1011
.	Non-Classical	16.5738	3.6217	16.6539	2.3747	28.7992	2.7827
3	Atomic Mix (Γ_1)	17.3804	8.6649	17.3804	6.8408	30.1038	7.4529
.	Atomic Mix (Γ_2)	14.8939	6.8811	14.8939	8.4442	25.7970	7.9329
.	Atomic Mix (Γ_3)	14.0990	11.8514	14.0990	13.3310	24.4201	12.8354

The estimated Monte Carlo errors are smaller than all the estimated Atomic Mix Model errors, and smaller than all but one of the estimated Non-Classical Theory errors. Thus, most of the errors in the Atomic Mix and Non-Classical estimates are due to modeling errors caused by the fact that the models do not perfectly reproduce the transport physics.

The choice of cross sections was such that Problem 2 is further away from the Atomic Mix limit than Problem 1, and Problem 3 even more so. This should cause the Atomic Mix estimates to be less accurate as we move from Problem 1 to Problem 2 and then to Problem 3. Moreover, the product $\Sigma_{t,1}\Sigma_{a,1}$ is the same in all problems; thus all problems have the same theoretical "diffusive" characteristics. More importantly, given a choice of $\langle \Gamma \rangle$, this causes the estimates of the Atomic Mix Model to be exactly the same for all three problems.

The Non-Classical Theory yields very accurate predictions of $\langle \rho^2 \rangle$, although it tends to slightly overestimate the mean-squared displacement. Its accuracy decreases by a factor of ≈ 3 for each new choice of cross sections; however, its accuracy in the prediction of the anisotropic behavior is remarkable, being a feature that does not exist in the Atomic Mix Model.

We can see that the Atomic Mix seems to work best when we choose an intermediary packing fraction like

$\langle \Gamma_2 \rangle$. Nonetheless, even in this case its accuracy fails to consistently match the accuracy demonstrated by the Non-Classical Theory. Clearly, a convenient choice for $\langle \Gamma \rangle$ will improve the accuracy obtained with this model. For this type of problem, however, there is no obvious procedure to make this choice in a non-artificial way. Furthermore, any particular choice of packing fraction will yield identical results for problems with the same theoretical "diffusive" characteristics. In other words, given a packing fraction, for problems in which the product $\langle \Sigma_t \rangle \langle \Sigma_a \rangle$ is the same, the Atomic Mix Model always predicts the same diffusion coefficient. Clearly this cannot be true, as we have shown here.

To summarize, the Non-Classical estimates for $\langle \rho^2 \rangle$ have about 1/6 the error of the best Atomic Mix estimate for Problem 1, about 1/2 the error of the best Atomic Mix estimate in Problem 2, and about 1/3 the error of the best Atomic Mix estimate in Problem 3. Moreover, the Non-Classical Theory accurately predicts the anisotropic behavior of the problems. The probable reason for the increased accuracy of the Non-Classical diffusion model is that it uses detailed physics properties of the random system that are not used in the simpler Atomic Mix approximation. For this reason, the Non-Classical asymptotic diffusion model will likely continue to be more accurate than the Atomic Mix solution for other "diffusive" neutron transport problems in random media.

4. CONCLUSION

In this work, we developed Monte Carlo codes that generate numerical results for certain microscopic and macroscopic quantities for neutron transport inside a simplified model 3-D PBR core. We focused our efforts on investigating the anisotropic diffusion of neutrons that are born close to a wall of this random system. Although this simplified model does not reflect the actual physical process encountered at the boundary of a PBR core, these results can be used to assess the accuracy of the Atomic Mix Model and the Non-Classical Theory in predicting this anisotropic diffusion.

We then proceeded to compare these Monte Carlo results with estimates obtained with the diffusion approximations of the Atomic Mix Model and of the Non-Classical Theory.

The diffusion approximation of the Non-Classical Theory is more costly to simulate than the Atomic Mix diffusion approximation. The Atomic Mix approximation only requires that one knows the cross sections of the constituent materials and their volume fractions; the Non-Classical Theory requires much more detailed information, which can be numerically obtained.

Nonetheless, because the Non-Classical Theory preserves certain statistical properties of the original random system, it represents a systematically more accurate alternative to the Atomic Mix approximation. In fact, in the problems proposed here, its estimates significantly outperform the ones obtained with the Atomic Mix Model. Moreover, it accurately predicts the anisotropic diffusion of the problems.

The present work paves the road to a formulation that may enable more accurate diffusion simulations of PBR cores to be performed in the future. By showing that the Non-Classical Theory outperforms the Atomic Mix Model in predicting anisotropic diffusion, one hopes that a method involving diffusion coefficients obtained with this theory will be an improvement over the current methods. To obtain such a formulation, the following steps should be performed:

I Space-dependent anisotropic diffusion coefficients must be calculated. (This is *not* what we have done in this paper; here, we have shown that the Non-Classical Theory accurately predicts the anisotropic

diffusion of neutrons caused by the arrangement of pebbles near the boundaries, proving it to be a useful tool to obtain these space-dependent anisotropic diffusion coefficients.)

II The anisotropic diffusion problem must be solved on a spatial grid sufficiently fine to account for the boundary effects.

Step **I** in this procedure requires careful attention, as it needs more detailed modeling of the PBR boundary to be performed.

For instance, in a cubic system like the one presented here, one could obtain space-dependent diffusion coefficients with the Atomic Mix Model by defining the packing fraction at depth x as the ensemble-averaged area of the pebbles sliced by the y, z-plane at depth x divided by L^2 (the area of the wall). Then, the ensemble-averaged packing fraction will increase (as x increases) from 0 at the wall $x = -L/2$ to the ensemble-averaged volumetric packing fraction in the interior of the system.

However, while previous work [1] has shown that anisotropic diffusion of neutrons is nearly neglectable in the interior of such a model PBR core, it has also shown that the diffusion coefficients obtained with the Non-Classical Theory are significantly more accurate than the ones obtained with the Atomic Mix approach [1,4,5]. Bearing this in mind, and taking the present work into account, it is our expectation that the possible gain in accuracy will prove the extra work worthwhile.

In other words, we do not (yet) claim that the Non-Classical Theory will yield significantly more accurate estimates of the eigenvalue and eigenfunction in a criticality calculation. However, we believe that this is an alternative to current methods that is worth pursuing.

In future work, we intend to improve the simplified model of the core used here in order to better reflect the physical process near the boundary of a PBR core, and then proceed to obtaining the space-dependent anisotropic diffusion coefficients.

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