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TREATMENT OF THE DOUBLE HETEROGENEITY WITH THE METHOD OF CHARACTERISTICS

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ABSTRACT

The problem of the double heterogeneity is modeled using an analytical asymptotic solution for a system of renewal equations describing transport in a stochastic mixture of grains diluted in a homogeneous matrix. The renewal equations have been obtained by truncature of an infinite hierarchy of integral equations, the truncature been exact at the limit of collisionless transport. The analytical solution used in this work has been developed for the case of a matrix with Markovian chord statistics, whereas an isotropic chord distribution is used for the grains assumed to be spherical. The solution is not valid in a boundary layer of the size of the grains, and this boundary error propagates into the inner solution resulting in loss of particle conservation. The model can be directly used in the solution by the method of characteristics (MOC) with a minimum implementation effort that does not affect the innermost calculation loop. A normalization condition has also been introduced to ensure conservation. This normalization is based on a modification of the cross section that describes particle streaming in the stochastic mixture. We have compared the behavior of this MOC treatment to an approximate model proposed in conjunction with the collision probability (CP) method a few years earlier. The comparisons were done for experiments carried out at the Physical Constants Testing Reactor and, because of the uncertainties of the 'measured' values, do not allow to decide which model is the best. However, the comparisons proof the validity of the MOC model that, contrary to the CP method, accounts for shadow effects due to the presence of more than one grain along a trajectory.

1. INTRODUCTION

Deterministic transport calculations require an exact description of the geometrical domain, i.e. a unique set of values of the cross sections must be assigned to each point in the domain. These methods cannot be directly applied to the calculation of a medium with a stochastic dispersion of components, such as UO_2 fuel with Gadolinia grains, or to a problem where the geometrical location of the different components is not exactly known, as in HTR pellet fuel. An approximate collision probability (CP) technique has been developed in the past to treat such type of 'double heterogeneity' problems. The first heterogeneity refers to the different regions of the calculation and the second refers to the internal structure of the stochastic components (grains) in a region. The CP treatment [1] consists of a pre homogenization of the regions comprising stochastic components (grains) based on the assumption that the angular flux entering and exiting the grains is uniform and isotropic.

A more correct manner to treat this problem is to utilize techniques based on the theory of transport in stochastic media. In a previous work [[1]] we have used renewal theory to obtain an analytical solution for a two-component stochastic medium comprising a matrix containing a dispersion of grains. This solution was used to analyze the approximate CP treatment and to obtain a better homogenization. However, the CP homogenization introduces an approximation that is not justified in the frame of stochastic analysis. In this work we have implemented the stochastic solution in the method of characteristics for unstructured geometries (MOC), providing thus for a solution that is free of homogenization effects.

This paper is organized as follows. In Section 2 we review transport in stochastic multicomponent media as applied to a renewal chord distribution and present an analytical solution appropriate for grain statistics. Briefly, we discuss multicomponent statistics, introduce the second-order closure for renewal chord statistics and discuss the analytical solution for grain statistics. In Section 3 we show how this analytical solution can be used in conjunction with the method of characteristics in the code TDT [[2]]. Our implementation is straightforward and does not require any fundamental structural changes in the code. We also show in this section how the asymptotic synthetic acceleration technique (ASA) can be generalized to treat stochastic grain components. Numerical results and comparisons with experimental values are presented in Section 4, while conclusions and discussion are given in Section 5.

2. RENEWAL EQUATIONS

The object of stochastic transport theory is to describe particle transport in a domain for which cross sections, sources and boundary conditions are known only in a statistical sense. To be more precise, a stochastic transport problem in a geometrical domain D is defined by a statistical set Ω, that comprises all possible physical realizations, together with a density of probability $p : \Omega \rightarrow R_+$. By a physical realization $\omega \in \Omega$ one understands a deterministic set of cross sections, sources and boundary conditions for which one can calculate an angular flux $\psi(x;\omega)$ solution of the transport problem. To set the ideas one may think of a domain comprising a statistical dispersion of microscopic grains. The mean number of grains per unit volume may be as large as 10^6 per cubic centimeter and the exact position of the grains is not known. Each deterministic distribution with a precise localization of the grains would correspond to a physical realization in the set Ω of all possible physical realizations. The probability of a given physical realization would depend on the process of fabrication. One would expect, for instance, that the probability for configurations that contain many grains stuck together would be small and, more generally, that the probability would be greater for grain distributions with small fluctuations on the mean number of grains per unit volume.

2.1 MULTIMATERIAL STATISTICS

Since the density of probability for each realization is known, one may in principle calculate the ensemble averaged angular flux,

$$\psi(x) = \int_\Omega \psi(x;\omega)p(\omega)d\omega,$$

but this requires, however, to compute a deterministic transport solution for each of the physical realizations. Such a computation is only possible if the number of realizations is finite. Hence, the first objective of stochastic transport theory is to obtain an equation of system of equations for the ensemble averaged solution for a statistical set containing an infinite number of physical realizations. Such a set of equations can be formally derived when the physical realizations are made up from a finite number of materials, where by a material we understand a mapping of the domain $\pi_i : D \rightarrow \{\Sigma, S\}$ that associates to each point a set of cross sections and sources and, for boundary points, a boundary condition. For such material statistics the ensemble average flux can be obtained as a weigthed sum of *material fluxes*:

$$\psi(x) = \sum_{i=1}^{i=M} p_i(x)\psi_i(x),$$

where M is the number of materials, $p_i(x)$ is the probability for material i at location x along a trajectory and where the material flux

$$\psi_i(x) = \int_{\Omega_i(x)} \psi(x;\omega)p(\omega)d\omega / \int_{\Omega_i(x)} p(\omega)d\omega \tag{1}$$

is the ensemble average of the angular flux for all realizations that have material i at point x.

For multimaterial statistics one can derive a system of equations for the material fluxes. This system is not closed because new ensemble averaged fluxes, called *transition fluxes*, appear as source terms. The transition fluxes originate in the process of ensemble averaging the transport equation to derive an equation for the material fluxes. As the point x moves along the trajectory the ensemble $\Omega_i(x)$ changes because some physical realizations leave the

ensemble and new ones enter it. The changes in $\Omega_i(x)$ appear as positive and negative sources in the transport-like equation for the material flux i. Before discussing the nature of transition fluxes we need to introduce the notion of a transition point. Given a physical realization $\omega \in \Omega$, a point x along a trajectory is called a transition point if the materials i_L and i_R at the left and at the right of x are different. The simplest material flux is defined as the ensemble average flux over all realizations that have a transition at a given location:

$$\psi_{ij}(x) = \int_{\Omega_{ij}(x)} \psi(x;\omega)p(\omega)d\omega / \int_{\Omega_i j(x)} p(\omega)d\omega, \tag{2}$$

where $\Omega_{ij}(x)$ is the subset of realizations that have the transition $i \rightarrow j$ at point x along the trajectory.

A new system of equations can be written for the transition fluxes but, again, higher ensemble averages are required. The result of this approach is an infinite hierarchy of equations that involves higher and increasingly singular flux ensemble averages. A truncation has to be introduced to obtain a workable model.

2.2 RENEWAL LINE STATISTIC

The truncation used in this work is exact for collisionless transport with renewal line statistics. To construct this statistics one assigns a density of probability $f_i(l)$ for the chord length l of each material and, in the case of more than two materials, a set of transition probabilities from each material to the others: $t_{ij}(x)$ = probability for a transition from material i into material j, given that there is a transition at x from material i into a different material. The associated line statistics are characterized by the fact that the distribution of materials to the right and left of a transition point are statistically independent.

The definition of the complete line statistics requires four conditional probabilities for each material. There are two probabilities conditioned to the fact that x is an interior point of material i:

- $R_i(l)$ = probability that material i spreads at least over a distance l to the right of point x,
- $g_i(l)$ = density of probability that material i reaches exactly a distance l to the right of point x,

and two similar probabilities but conditioned to the fact that x is a transition point into material i:

- $Q_i(l)$ = probability that material i spreads at least over a distance l to the right of point x,
- $f_i(l)$ = density of probability that material i reaches exactly a distance l to the right of point x.

All these quantities are not independent because of the obvious relations:

$$g_i(l) = -\partial_l R_i(l),\ f_l(l) = -\partial_l Q_i(l)$$

that, together with the initial values $R_i(0) = Q_i(0) = 1$, allow to compute the probabilities from the respective densities of probability.

These four probabilities as well as the transition probabilities between materials may depend on the position x along the trajectory as well as on the orientation of the trajectory. However, in this work we exclusively consider homogeneous statistics, i.e., statistics that are invariant under translations and symmetries. For this statistics the different probabilities do not depend neither on position nor on orientation [[3]]. Moreover, for homogeneous chord statistics all chord probabilities can be obtained from the density of probability for the chord length, $f_i(l)$ via the relation $g_i(l) = Q_i(l)/\lambda_i$, where λ_i is the mean chord length in material i. Therefore, a complete definition of homogeneous, renewal line statistics requires only the values of the transition probabilities t_{ij} and of the chord length densities of probability $f_i(l)$ for each material i.

A particular type of renewal line statistics is Markovian statistics for which right and left material distributions are statistically independent at any position x, regardless of whether x is in the interior of a material or is a transition point. Markovian statistics require exponential chord length distributions for all materials: $f_i(l) = \exp(-l/\lambda_i)/\lambda_i$.

2.3 SECOND-ORDER RENEWAL CLOSURE

Equations for the material fluxes can be obtained by ensemble averaging of either the integrodifferential transport equation of the integral form of the transport equation. The lowest-order renewal equations for renewal statistics are derived from the integral form of the transport equation. For collisionless transport this equation reads:

$$\psi_i(x) = e^{-\tau_i(0,x)} R_i(x)\psi_{in} + \int_0^x [R_i(x-y)q_i(y) + g_i(x-y)\psi_i^{in}(y)]e^{-\tau_i(y,x)}dy, \tag{3}$$

where $\tau_i(y,x)$ denotes the optical distance in material i between positions y and x. The first term on the right hand side represents the uncollided neutrons entering the domain at $x = 0$, while the second term contains the contributions from the internal sources in material i, q_i, and from the boundary fluxes at transitions from a different material into material i, ψ_i^{in}. In this equation and in the following we assume that the boundary condition ψ_{in} is independent of the physical realization.

The transition flux $\psi_i^{in}(x)$ entering material i at x is the statistical average for all realization that transit into i at that location. Therefore it can be written as the contributions from the transition fluxes leaving the other materials

$$\psi_i^{in}(x) = \sum_{j \neq i} t_{ij}\psi_j^{out}(x), \tag{4}$$

The transition fluxes themselves are also given by equations similar to (3). For collisionless transport these equations constitute a closed system for all the transition fluxes:

$$\psi_i^{out}(x) = e^{-\tau_i(0,x)} Q_i(x)\psi_{in} + \int_0^x [Q_i(x-y)q_i(y) + f_i(x-y)\psi_i^{in}(y)]e^{-\tau_i(y,x)}dy. \tag{5}$$

System of Eqs. (3)-(5) form a closed system for the calculation of the material fluxes and, therefore, of the ensemble average flux. Once the transition fluxes are obtained from Eqs. (5), their values can be used in (3) to compute the material fluxes. The second-order renewal closure is to apply these equations to the case of collisions. Numerical tests have shown the validity of this closure.

2.4 ANALYTICAL SOLUTION FOR GRAIN STATISTICS

The problem we want to consider is that of a stochastic dispersion of grains in a homogeneous matrix. We adopt renewal line statistics and consider that there are M types of different grains with given chord lengths distributions. In the following we will use the index 0 to denote the matrix and the index i, from 1 to M, to indicate the different grains.

In order to obtain an analytical solution we assume that the grains do not collapse and that the matrix follows Markovian chord statistics, $f_0(l) = \exp(-l/\lambda_0)/\lambda_0$. We take the grains to be spherical in shape and consider the grains as multilayered one-dimensional spheres. Then an asymptotic solution of Eqs. (3) is [[1]]:

$$\left.\begin{array}{c} \psi_0^{out}(x) = e^{-\Sigma x}\psi_{in} + (1 - e^{-\Sigma x})\psi_{as} \\ \psi_i^{out}(x) = e^{-\Sigma x}\psi_{in}\widehat{T}_i^g + (T_i^g - e^{-\Sigma x}\widehat{T}_i^g)\psi_{as} + \psi_i^{out} \end{array}\right\}, \tag{6}$$

where

$$\left.\begin{array}{c}\psi_{as} = (q_0 + \frac{1}{\lambda_0}\sum_i t_i \psi_i^{out})/\widetilde{\Sigma} \\ \psi_i^{out} = \lambda_i \sum_k p_{ik}^g q_{ik} E_{ik}^g \end{array}\right\}$$

with $p_0 =$ volumetric fraction for matrix, $p_i =$ volumetric fraction for grain i, $p_{ik}^g =$ volumetric fraction for layer k of grain i, $\lambda_i =$ average chord length for grain i, $q_0 =$ angular emission in the matrix, $q_{ik} =$ angular emission in laker k of grain i, $T_i^g =$ transmission probability for grain i, $\widehat{T}_i^g =$ transmission probability for grain i with the total cross section diminished by Σ, $E_{ik}^g =$ escape probability from layer k of grain i, and the cross sections:

$$\left.\begin{array}{c}\widetilde{\Sigma} = \Sigma_0 + \frac{1}{\lambda_0}\sum_i t_i (1 - T_i^g) \\ \Sigma = \Sigma_0 + \frac{1}{\lambda_0}\sum_i t_i (1 - \widehat{T}_i^g) \end{array}\right\}. \tag{7}$$

This last equation is a nonlinear equation that implicitly defines Σ. Moreover, $t_i = (\lambda_0 p_i)/(p_0 \lambda_i) =$ transition probability from matrix into grain i.

Because the matrix follows Markovian chord length statistics, the material flux for the matrix equals the transition flux, $\psi_0(x) = \psi_0^{out}(x)$. The solution for the material fluxes in the grains is:

$$\psi_{ik}(x) = e^{-\Sigma x}\psi_{in}\widehat{E}_{ik}^g + [E_{ik}^g - e^{-\Sigma x}\widehat{E}_{ik}^g]\psi_{as} + \psi_{ik}, \tag{8}$$

where $\widehat{E}_{ik}^g =$ escape probability from layer k of grain i with the total cross section diminished by Σ and

$$\psi_{ik} = \frac{1}{V_{ik}^g \Sigma_{ik}} \sum_l V_{il}^g q_{il} P_{ik;il}^g$$

with $V_{ik}^g =$ volume of layer k of grain i and $P_{ik;il}^g =$collision probability from layer l to layer k within grain i.

The analytical solution in (6) and (8) is asymptotic because it is not valid in the boundary layer of thickness $\delta = 2\max_i R_i$, where R_i is the external radius of grain i. For the interior solution to be exact the ψ_{in} in (6) and (8) should be the value of the material flux ψ_0 at $x = \delta$. The later material flux could be obtained, in principle, by matching the interior solution with the boundary layer one. However, the solution across the boundary layer cannot be obtained in a closed form and we prefer to assume that Eqs. (6) and (8) apply throughout the boundary layer.

3. NUMERICAL IMPLEMENTATION

The analytical solution for renewal grain statistics just described can be used to implement a numerical solution with the method of characteristics for unstructured meshes (MOC) containing regions with stochatics materials.

3.1 THE METHOD OF CHARACTERISTICS

The iterative solution for the MOC is based on a conservation and a transmission equation along each trajectory crossing a region. These are exact equations based on the assumption that the sources and cross sections are uniform within the region:

$$\left.\begin{array}{c}\psi_+ = (1 - \Sigma\beta)\psi_- + \beta q \\ \psi_+ - \psi_- + \Sigma L \overline{\psi} = Lq \end{array}\right\}. \tag{9}$$

Here ψ_+ and ψ_- are the outgoing and incoming fluxes along the trajectory, L is the length of trajectory intersected by the region, ψ the mean flux over this length, q the cell average source, Σ the total cross section and $\beta = [1 - \exp(-\Sigma L)]/\Sigma$ the region transmission coefficient along the trajectory.

The first equation in (9) gives the outgoing flux in terms of the incoming one and from the value of the source from the previous iteration. The second equation yields the average flux over the chord intersected by the trajectory.

These chord averages are used at the end of the iteration to compute cell average values,

$$\overline{\psi}_{cell}(\mathbf{\Omega}) = \frac{1}{V}\sum_{t//\mathbf{\Omega}} w_{\perp}(t,\mathbf{\Omega})\int_0^{L(t,\mathbf{\Omega})} dx\psi(x) = \frac{1}{V}\sum_{t//\mathbf{\Omega}} w_{\perp}(t,\mathbf{\Omega})(L\overline{\psi})(t,\mathbf{\Omega}), \tag{10}$$

that are then used to estimate new averaged cell sources for the next iteration. The sum in (10) is done for all trajectories t with direction $\mathbf{\Omega}$ that intersect the cell, V is the cell volume and $w_{\perp}$ is the angular quadrature weight times the trajectory cross section.

3.2 TREATMENT OF THE DOUBLE HETEROGENEITY

In order to extend the MOC equations to the treatment of a stochastic region we need to estimate ψ_+ as the ensemble averaged angular flux exiting the region along the trajectory. We assume that grains are contained in the interior of the region and that, therefore, cannot cross its boundaries. This means that ψ_+ can be identified with the material flux in the matrix. The analytical solution for $\psi_0^{out}(x)$ in (6) can be rewritten in a way similar to the MOC transmission equation in (9):

$$\psi_+ = (1-\Sigma\beta)\psi_- + \beta q, \tag{11}$$

where $q = \Sigma\psi_{as}$ is the effective source in the stochastic region and β the transmission factor computed now with the stochastic cross section Σ defined in the second equation of (7). Note that the boundary incoming flux ψ_{in} in (6) and (8) must be identified with the incoming cell flux ψ_-.

The next step is to establish equations for the calculation of the cell average fluxes for the matrix and for the different type of grains contained in the matrix. The average values over the intersection of the trajectory with the region can be obtained by integration over the chord of the material fluxes given in (6) and (8). The resulting equation for $\overline{\psi}_0$ can be written in the form of a balance equation as in (9):

$$\psi_+ - \psi_- + \Sigma L\overline{\psi}_0 = Lq, \tag{12}$$

whereas the mean chord flux for the grains can be written in terms of $\overline{\psi}_0$:

$$\overline{\psi}_{ik} = \widehat{E}_{ik}^g\overline{\psi}_0 + (E_{ik}^g - \widehat{E}_{ik}^g)\psi_{as} + \psi_{ik}. \tag{13}$$

At this point we note that thanks to Eqs. (11) and (12) we can implement the sweep trough a stochastic region without need of modifying the programmation for the MOC done for the case of homogeneous regions containing deterministic materials. The only difference consists of calculating the effective source $q = \Sigma\psi_{as}$ before each iteration. Further, at the end of the iteration we may compute the updated mean flux in the grains as:

$$\overline{\psi}_{ik,cell}(\mathbf{\Omega}) = \widehat{E}_{ik}^g\overline{\psi}_{0,cell}(\mathbf{\Omega}) + (E_{ik}^g - \widehat{E}_{ik}^g)\psi_{as}(\mathbf{\Omega}) + \psi_{ik}(\mathbf{\Omega}).$$

The interest of this implementation is that it requires small program modifications, just before and after the sweep, hence the internal sweep is not modified.

3.3 ENFORCING CONSERVATION

A problem with the treatment of the double heterogeneity just discussed is that the resulting equations are not conservative. The lack of conservation stems from the fact that the stochastic solution is not valid throughout the boundary layer and, therefore, does not match correctly the incoming flux at the cell boundary. Further, the error made in the boundary layer propagates to the interior solution and the result is that the local conservation equation is not satisfied even in the interior of the region.

This entails that our final equations are not conservative and we found after some amount of algebra, that the net production along a trajectory is:

$$\begin{aligned} Production &= \int_0^L dx\{p_0[q_0 - \Sigma_0\psi_0(x)] + \sum_i p_i \sum_k p_{ik}^g[q_{ik} - \Sigma_{ik}\psi_{ik}(x)]\} \\ &= f(\psi_{as} - \psi_{in})\beta, \end{aligned}$$

where we have used the definitions for ψ_{as} and $\widetilde{\Sigma}$ and

$$f = p_0\Sigma_0 + \sum_i p_i \sum_k p_{ik}^g \Sigma_{ik}\psi_{ik}E_{ik}^g. \tag{14}$$

On the other hand the total leakage is

$$Leakage = \psi_{out} - \psi_{in} = (\psi_{as} - \psi_{in})\beta.$$

To ensure particle conservation we must have $\Sigma = f$ instead of the stochastic value of Σ implicitly defined in (7). In our work we have chosen to use the value in (7) to compute the coefficients $\widehat{E}_{ik}^g$ and then to use the new value given by $\Sigma = f$ in the method of characteristics. In such a way the stochastic value for Σ is used to compute the effective source and the propagation of neutrons between matrix and grains, while the new value $\Sigma = f$ is used for propagation along the trajectory enforcing, thus, particle conservation in the region.

We may calculate the new value of Σ given by (14) from the equivalent formula:

$$\Sigma = (p_0 + \sum_i p_i \sum_k p_{ik}^g \widehat{E}_{ik}^g)\Sigma^{old}, \tag{15}$$

where Σ^{old} denotes the value given by (7). This formula shows that when the grains and the matrix have the same total cross section the new value for Σ equals the old one. For grains that are more absorbant than the matrix, the result amounts to an increase of the transparency of the region by a value between p_0 and 1, while in the opposite case the medium become less transparent.

4. EXAMPLE CALCULATION

We have used the new functionalities of the MOC method to analyze the set of experiments conducted at the Physical Constants Testing Reactor (PCTR) [[4]]. In this experiments a sample of a stochastic material containing PuO_2 grains was put in the center of a test lattice and the k_∞ was then inferred from the Boron concentration needed to ensure criticality. A series of experiments provided k_∞ values for different grain sizes and Pu mass proportions in the absence and in the presence of Boron.

Because of the difficulties of obtaining the exact lattice description we have considered only a periodic lattice generated from one of the square cells in the sample. We have run 172-group 2D calculations with a total of 43 regions (6 fuel regions, with 4 regions per grain, 1 clad region and 13 moderator regions) for the different grain sizes, Pu mass proportions and final Boron concentrations in the experiment. Because we could not calculate the entire lattice (not enough experimental data), we cannot compare directly the k_∞ values. Also, the fact that the calculations depend on three different parameters, makes comparisons very difficult because of the measurement uncertainties. However , the comparison of the linear regression for the k_∞ data compared in Table1 to the experimental results for grains with the same Pu mass and without Boron shows that our results predict the slope within the uncertainties of experimental results. The detailed values for these calculations are given in Table 2 and in Figure 1. 10^{-5}

Given the uncertainty in the measured values both slopes, as predicted by the CP and the MOC calculations, are within experimental errors and this comparison does not permit to decide which method is better. The comparison confirms, however, that the MOC values are not erroneous.

Experiment	CP	MOC
1.30842-14.673 $10^{-5}\times$D	1.36637-11.443 $10^{-5}\times$D	1.32852-11.062 $10^{-5}\times$D

Table 1. Linear regression for k_∞ versus grain diameter D. CP = collision probability calculations with homogenized cross sections. MOC = characteristic calculation with stochastic solution

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$D_g[\mu$m]	k_∞(experiment)	k_∞ (CP)	k_∞(MOC)	$\varepsilon(CP)$	ε(MOC)
0.1	1.31467±0.005	1.36652	1.32828	3943	1010
52	1.30300±0.005	1.36019	1.32275	4389	1015
107	1.27933±0.005	1.35395	1.31680	5833	2929
195	1.28200±0.005	1.34439	1.30708	4867	1956
328	1.26300±0.005	1.32872	1.29213	5203	1023

Table 2. CP and MOC k_∞ results for the cases without Boron. The errors in columns 5 and 6 are given in pcm (1 pcm = 10^{-5}).

In Table 3 we give comparative results for all the experimental values for grains with borated water. Unfortunately, these cases differ in the values of three experimental parameters, grain size, Pu mass and Boron concentration, and, given experimental errors, it is not possible to extract any useful information, except that both the CP and the MOC predict sensible values for the k_∞.

$D_g[\mu$m]	$\rho_{\text{fuel.}}$	PuO_2 mass (%)	Boron	K_∞[exp.]	K_∞ (CP)	K_∞(MOC)
0.0	8.704	2.08	1286±4	0.991	1.00630	0.97258
0.0	8.474	2.10	1274±4	0.992	1.00489	0.97489
25	9.540	2.00	1353±4	0.995	0.99955	0.96447
52	8.601	2.29	1350±4	0.992	1.00680	0.97210
107	8.739	2.48	1378±4	0.991	1.01657	0.98170
107	8.638	2.47	1332±4	0.997	1.02180	0.98695
107	7.630	2.45	1227±4	0.989	1.01331	0.97969
195	8.718	2.35	1275±4	0.995	1.00892	0.97399
195	8.657	2.41	1261±4	0.985	1.01677	0.98173
328	8.691	2.42	1163±4	0.992	1.01823	0.98343
328	8.798	2.47	1229±4	0.984	1.01230	0.97744

Table 3. CP and MOC k_∞ results for the cases with Boron. The density is in grams per cubic centimeter. The Boron concentration is in pcm (1 pcm = 10^{-5}).

5. CONCLUSION

A stochastic solution for a multicomponent renewal transport process has been used to calculate mean cell and region fluxes in the method of characteristics for unstructured meshes. Contrarily to the collision probability double-heterogeneity method, this solution does not require a pre homogenization of the stochastic components. An efficient acceleration algorithm has been developed by using the basic assumptions of the ASA acceleration previously developed for homogeneous regions.

We have presented some of our results for the analysis of the PCTR experiments for the case of non-borated water and compared these with results obtained from the collision probability method by pre homogenization of the stochastic regions. Because of the experimental uncertainties it is not possible to decide weather the CP approach or the MOC are better, and it could be that the MOC may be better in some range of parameters (grain sizes and

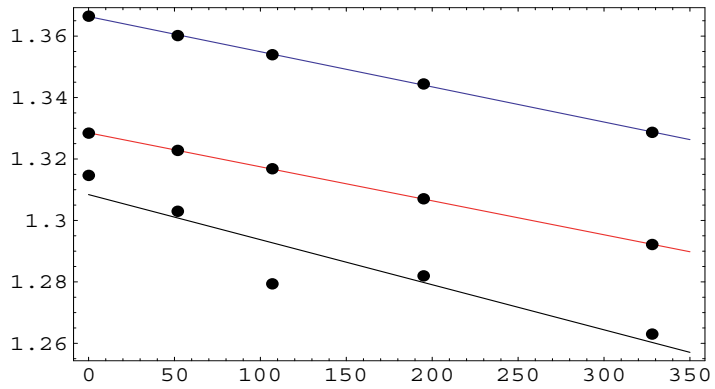

Fig. 1. k_∞ versus grain diameter. Lower curve: experiment. Middle curve (red): characteristics calculation with stochastic solution. Upper curve (blue): collision probability calculations with homogenized cross sections.

cross sections, relative mass of grains in the matrix) and the CP better in the complementary range. We recall here that the CP treatment is based on a dubious homogenization that preserves the transmission probability of the region for uncollided neutrons for an isotropic and uniform incoming angular flux. Moreover, in the process of homogenization, the calculation of the transmission probability for the stochastic medium is done by neglecting shadow effects, i.e., by assuming that there is only one grain that intersects the trajectory. In contrast, the MOC treatment is based in a direct solution of the stochastic problem and does not require a homogenization. Unfortunately, the solution is not conservative and requires the introduction of and ad-hoc cross section that is then used for propagation across the region.

The stochastic analytical solution is not valid through a boundary layer of width of the size of the grains diameters. Since the direct use of the stochastic analytical solution results in a non conservative characteristics scheme, we have redefined a new cross section for use in cell propagation that enforces conservation. In all our tests calculations we have observed that the 'conservative' cross sections does not differ much from the stochastic cross section. For the results presented here for the MOX experiments both cross sections were nearly identical. For other calculations done for UO_2 fuel poisoned with Gadolinia grains the conservative cross sections can be as small as 80% of the stochastic cross section. Work remains to be done to analyze in depth the problem of conservation and, if possible, use an approximate solution through the boundary layer to better match the entering angular flux. The constraint is that too strong a modification of the approximate analytical solution may demand an deep change in the internal sweep for the method of characteristics, requiring thus a more complicated implementation.

A basic difficulty with the validation of the new traitement of the double heterogeneity problem with the MOC is the absence of precise enough experimental data. In the future we intend to exploit concentration measurements obtained after irradiation of poisoned UO_2 fuel with Gadolina grains.

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