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Renormalized treatment of the double heterogeneity with the method of characteristics

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A numerical solution for the method of characteristics in structured meshes is proposed to treat media comprising stochastic regions. As opposed to an earlier approach, the new method uses the stochastic solution predicted by renewal theory to compute region transmission and a normalizing coefficient is applied then to ensure conservation. Numerical comparisons are presented for set of Kritzs experiments for MOX fuel, and for a 2D HTGR reactor with prismatic fuel elements. Comparisons with a Monte Carlo calculation show that the renormalized MOC treatment predicts assembly powers within 1%.

KEYWORDS: double heterogeneity, method of characteristics, numerical methods, HTGR

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 the past [1] we have used renewal theory to obtain an asymptotic analytical solution for a multi-component stochastic medium comprising a matrix containing a dispersion of spherical grains. This solution, which depends on a stochastically defined cross section Σ, was used to analyze the approximate CP treatment and to obtain a better homogenization. The advantage of the double heterogeneity CP approach is that the use of the homogenized cross sections allows a full treatment of a domain comprising deterministic and stochastic regions, and this including flux reconstruction in the different components of each stochastic region. However, to achieve this both CP methods assume that neutrons enter the regions in an isotropic and uniform way,[1] and therefore make a drastic simplification for the interaction between the different regions of the domain.

In a previous work [3] we have implemented the asymptotic stochastic solution in the method of characteristics for unstructured geometries (MOC),[2] providing thus for a solution that is free of homogenization effects. The interest of this approach was to offer a direct deterministic treatment for a domain containing homogeneous regions as well as regions comprising a statistical dispersion of micro particles in a homogenous matrix. Another advantage of the proposed method was that the numerical efficiency of the MOC was not affected because the asymptotic analytical solution of the stochastic renewal equations did not require a modification of the inner sweeping loop. However, a drawback with the work presented in [3] was that the analytical asymptotic solution is not valid in a boundary layer and that, therefore, it cannot match exactly the boundary condition. For a path of length l across a stochastic region this results in the following conservation relation:

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

where

$$r = \Sigma_c/\Sigma, \tag{2}$$

Σ_c is a new stochastically defined cross section, ψ_+ and ψ_- are the angular fluxes exiting and entering the path, q is a source term that depends on the asymptotic stochastic solution, and

$$\beta = [1 - \exp(-\Sigma l)]/\Sigma \tag{3}$$

is the escape probability associated to cross section Σ. The factor r in Eq. (1) is required to ensure conservation, such that $r\beta(q - \Sigma\psi_-)$ equals the difference $sources - collisions$ across the chord of length l of the stochastic region. This factor comes about because the asymptotic solution is only good far from boundaries and therefore cannot match the boundary condition $\psi = \psi_-$ at the beginning of the chord.

With the exception of the factor r, Eq. (1) looks like the typical conservation equation used for a homogenous region in the MOC. In our previous work [3] we decided to replace Σ with Σ_c, therefore artificially setting r to 1, in order to embed the stochastic solution in the MOC's numerical implementation. However, this entailed using a different stochastic behavior than the one predicted by the stochastic solution (use of Σ_c instead of Σ to compute the escape probability β.) Although in all cases considered in [3] we found $\Sigma_c/\Sigma \approx 1$, this implementation was felt unsatisfactory because it did not preserve the behavior of true stochastic propagation. It was observed, in particular, that when the grains are much more absorbing that the matrix the ratio r can be quite different from 1, attaining values of 0.95 and lower for UO_2 poisoned fuel.

In this work we have decided to keep the stochastic cross section to compute neutron propagation along the path and use the ratio r as a renormalization factor for the escape probability. Therefore, we write Eq. (1) as in the MOC method:

$$\psi_+ = \psi_- + \beta_c(q - \Sigma\psi_-), \tag{4}$$

where $\beta_c = r\beta$ and β is computed with the original Σ, respecting thus the true structure of the stochastic solution for the renewal equations. The factor r is introduced as a means to ensure conservation while preserving the stochastic asymptotic solution throughout the region.

In the next section we develop the characteristic equations for the new formulation and compare it with the ad-hoc correction done in our previous work. [3] We then analyze the implications of Eq. (4) and give a discussion of the physical interpretation of the stochastic cross sections Σ and Σ_c, and a comparative analysis of both normalizations with emphasis in their behavior in limiting situations.

In Section 3 we present our numerical results. We have repeated all the calculations for the Kritz experiments [4] and obtained qualitatively the same behavior than with our previous formulation. The reason is that for MOX fuel the ratio r is very close to 1 (the maximum deviation with our 180-group library was of 0.001) and therefore the two MOC formulations are close to each other. In the last part of Section 3 we present a comparison with a Monte Carlo calculation for the case of a HTR with prismatic fuel elements. [5] Conclusions are given in the last section. Finally, as with for the previous double-heterogeneity MOC formulation, the synthetic acceleration developed for the MOC [2] can be easily extended to treat the renormalized double-heterogeneity MOC formulation.[6] A brief survey of the equations is presented in the appendix.

2 Renormalized treatment for the MOC

The method of characteristic in unstructured meshes implements the iterative solution of the discrete ordinate formulation of the one-group transport equation for a piecewise homogeneous domain by using a) a flat source approximation and b) a set of parallel trajectories for each angular direction in the discrete ordinate set. At each iteration the integral transport equation is used compute the angular flux along each trajectory in terms of the incoming boundary flux and the sources form the previous iteration. Across a homogenous chord:

$$\psi_+ = \psi_- + \beta(q - \Sigma\psi_-), \tag{5}$$

where ψ_+ (ψ_-) is the angular flux exiting (entering) the homogeneous region of cross section Σ, q is the constant region source and β is the escape probability associated to a constant source distribution along the chord and given in (3). The escape probability, as well as the source q and the angular fluxes, ψ_+ and ψ_-, depend on the trajectory t and, therefore, on the angular direction $\mathbf{\Omega}$.

To update the source one needs to estimate the region-averaged angular fluxes:

$$V\psi_{reg} = \int_{reg} \psi d\mathbf{r} \sim \sum_t w_\perp l\overline{\psi}.$$

In this expression ψ_{reg} is the mean angular flux in the region, V is the volume of the region, the sum is done over all trajectories t that cross the region in direction $\mathbf{\Omega}$, l is the chord length across the region and $\overline{\psi}$ is the averaged angular flux along the chord:

$$l\overline{\psi} = \beta\psi_- + \frac{l-\beta}{\Sigma}q \tag{6}$$

With the help of this formula we can write

$$\psi_{reg} = \frac{1}{V}\Delta + \Pi q, \tag{7}$$

where

$$\Delta = \sum_t w_\perp \beta\psi_- \tag{8}$$

is to the sum of contributions of the trajectories that cross the region during a sweep, and

$$\Pi = \frac{1}{\Sigma}(1 - \frac{1}{V}\sum_t w_\perp\beta) \tag{9}$$

is independent of the sources and can therefore be precomputed.

The sources q are calculated prior to each power iteration, while the sweep along each trajectory is done in the inner loop of the MOC calculation. In order to speed up calculations the escape coefficients β are computed at the beginning of all the iterations for a given group, so that only two calculations are repeated in the inner loop. First, the exiting angular flux is computed from Eq. (5) and then the value of Δ, set to 0 prior to the sweep, is updated by the amount $w_\perp \beta \psi_-$.

2.1 Treatment of stochastic regions

We consider a stochastic region comprising a statistical dispersion of different types of microscopic grains in a homogeneous matrix. By using a renewal description of multimaterial statistics [1] for non collapsing grains and a Markovian chord distribution for the matrix one can derive an analytical expression for the asymptotic ensemble averaged fluxes along a chord:[1]

$$\left.\begin{array}{c} \psi_0(x) = e^{-\Sigma x}\psi_- + (1-e^{-\Sigma x})\psi_{as} \\ \psi_{ik}(x) = e^{-\Sigma x}\psi_- \widehat{E}_{ik} + [E_{ik} - e^{-\Sigma x}\widehat{E}_{ik}]\psi_{as} + \psi_{ik}, \end{array}\right\}, \tag{10}$$

where ψ_- is the incoming angular flux, x denotes the position along the chord, we have used the lower indexes 0 and ik to indicate the matrix and the layer k of grain type i, the E_{ik} is the escape probability from layer ik and $\widehat{E}_{ik}$ is the escape probability for a grain with the total cross section diminished by Σ. Also, in this equation ψ_{as} is the asymptotic flux in the matrix and ψ_{ik} is the average flux inside a grain due to its internal sources:

$$\left.\begin{array}{c} p_0\widetilde{\Sigma}\psi_{as} = p_0 q_0 + \sum_{i,k} p_{ik} q_{ik} E_{ik} \\ p_{ik}\Sigma_{ik}\psi_{ik} = \sum_l p_{il} q_{il} P_{ik,il} \end{array}\right\}, \tag{11}$$

where p_0 and p_{ik} are the volumetric proportions of matrix and layers so that $p_0 + \sum_{i,k} p_{ik} = 1$, q denotes the internal sources and $P_{ik,il}$ is the collision probability from layer l to layer k in a grain of type i.

Finally, in Eqs. (10) and (11) we have introduced the cross section $\widetilde{\Sigma}$ and the stochastic cross section Σ:

$$\left.\begin{array}{c} p_0\widetilde{\Sigma} = p_0\Sigma_0 + \sum_{i,k} p_{ik}\Sigma_{ik}E_{ik} \\ p_0\Sigma = p_0\Sigma_0 + \sum_{i,k} p_{ik}\widehat{\Sigma}_{ik}\widehat{E}_{ik} \end{array}\right\}, \tag{12}$$

where $\widehat{\Sigma}_{ik} = \Sigma_{ik} - \Sigma$. Note that the last equation defines Σ implicitly.

A word of caution must be said in regard to the asymptotic solutions in (10). To begin with these are the expressions for ensemble-averaged fluxes in the interior of the matrix and of the grains. Here 'ensemble-averaged' means the statistical average for all the physical realizations that have the given material present at position x. It is not the flux for the actual physical realization but an averaged flux over all the potential realizations. Moreover, the equations that have been used to obtain these asymptotic solutions are exact for collisionless transport and only an approximation when collisions are present. However, this approximation, that amounts to neglect correlations due to collisions, has been shown to hold for a large number of physical configurations with errors smaller than ten percent. Finally, the solutions in (10) are asymptotic in the sense that they do not satisfy the boundary condition. Indeed, on one hand one assumes that chord statistics are invariant by translations [7] and on the other the solution for the grains is only valid out of a boundary layer of thickness the maximum width of the grains.[1] Another way to see this is to realize that, although the flux in the matrix ψ_0 satisfies the incoming boundary condition at $x = 0$, the grain flux ψ_{ik} depends on the internal sources at any position x.

2.2 Implementation in the MOC

Our approximation is to consider that the asymptotic solution in (10) holds in the entire track across the region. We expect this assumption to work for regions of a fair size as compared to grain dimensions. Hence, the chord averaged angular fluxes in the matrix and in the layers, $\overline{\psi}_0$ and $\overline{\psi}_{ik}$, can be computed from (10) as:

$$\left.\begin{array}{c} l\overline{\psi}_0 = \beta\psi_- + (l-\beta)\psi_{as} \\ \overline{\psi}_{ik} = \widehat{E}_{ik}\overline{\psi}_0 + (E_{ik} - \widehat{E}_{ik})\psi_{as} + \psi_{ik} \end{array}\right\}. \tag{13}$$

Next, by adding the chord contributions for all trajectories crossing the region in a given angular direction we obtain the corresponding expressions for the cell-averaged fluxes:

$$\left.\begin{array}{c} \psi_{0,cell} = \frac{1}{V}\Delta + \Pi q \\ \psi_{ik,cell} = \widehat{E}_{ik}\psi_{0,cell} + \frac{E_{ik}-\widehat{E}_{ik}}{\Sigma} q + \psi_{ik} \end{array}\right\}, \tag{14}$$

where Δ and Π are those in (8) and (9), and where we have introduced the asymptotic source:

$$q = \Sigma\psi_{as} \tag{15}$$

To complete the formalism it remains to determine the angular flux ψ_+ exiting the chord. We obtain it from conservation by adding to the entering flux the sources emitted in the chord by the stochastic materials and by substracting the collisions with the different stochastic components:

$$\psi_+ = \psi_- + l[p_0(q_0 - \Sigma_0\overline{\psi}_0) + \sum_{i,k} p_{ik}(q_{ik} - \Sigma_{ik}\overline{\psi}_{ik})].$$

With the help of (13) the last equation results in (1) with Σ_c defined as:

$$\Sigma_c = p_0\Sigma_0 + \sum_{i,k} p_{ik}\Sigma_{ik}\widehat{E}_{ik}. \tag{16}$$

Then in order to run the inner MOC loop without any modification, it suffices to use (15) to construct the source in the stochastic regions and to replace β by $\beta_c = r\beta$ with the r of (2). Notice that this does not change the inner loop because the escape coefficients are computed prior to all group iterations. However, this entails that in the inner loop one computes the sum of $rw_\perp\beta\psi_-$ instead of $w_\perp\beta\psi_-$. Since it is the latter quantity that we require to calculate the cell averaged matrix flux in (14), we need to multiply by r^{-1} after the loop to recover the quantity of interest.

2.3 Limiting behavior

We investigate here the behavior of the solution in some limit situations.

By writing the sums over the layers in terms of grain transmission probabilities the cross sections $\widetilde{\Sigma}$ and Σ in Eq. (12) we obtain:

$$\left.\begin{array}{c} \widetilde{\Sigma} = \Sigma_0 + \sum_i \frac{p_i}{\lambda_i}(1 - T_i) \\ \Sigma = \Sigma_0 + \sum_i \frac{p_i}{\lambda_i}(1 - \widehat{T}_i) \end{array}\right\},$$

where p_i is the volumetric proportion of grains of type i, λ_i is the mean chord length T_i is the grain transmission probability and $\widehat{T}_i$ is the transmission probability for a grain with the cross section

diminished by Σ. From these expressions it can be easily checked that $\Sigma_0 \leq \widetilde{\Sigma} \leq \Sigma_0 + 1/\lambda_0$, $\widetilde{\Sigma} \leq \Sigma$ and that Σ obeys the following bounds:[1]

$$\min_{ik}(\Sigma_0, \Sigma_{ik}) \leq \Sigma \leq \min[\Sigma_0 + \frac{1}{\lambda_0}, \max_{ik}(\Sigma_0, \Sigma_{ik})]$$

having used $p_0/\lambda_0 = \sum_i (p_i/\lambda_i)$. This last formula determines the search range for the calculation of the Σ by iterative solution of nonlinear equation (12).

To complete our analysis we use (16) and (12) to write the renormalization ratio as follows:

$$r = \frac{\Sigma_c}{\Sigma} = p_0 + \sum_{i,k} p_{ik} \widehat{E}_{ik}.$$

We consider first the *homogeneous* limit when $\Sigma_{ik} \to \Sigma_0$ and $q_{ik} \to q_0$. We find that $\Sigma, \Sigma_c \to \Sigma_0$ and that $\psi_{ik,cell} \to \psi_{0,cell}$. Then, accounting for the fact that $q = \Sigma\psi_{as} \to q_0$ we find that all the cell averaged fluxes for matrix and layers are equal to the cell averaged flux one would have obtained had been the region homogeneous with cross section Σ_0 and source q_0.

Another important case is the so-called *atomic-mix* limit at which the grains become infinitesimally small, $\lambda_i \to 0$. Here we find $p_0\widetilde{\Sigma}, \Sigma, \Sigma_c \to \Sigma_{mix}$ and $q = \Sigma\psi_{as} \to q_{mix}$, where Σ_{mix} and q_{mix} are the total cross section and source of the volume-homogenized stochastic mixture:

$$\left.\begin{array}{c} \Sigma_{mix} = p_0\Sigma_0 + \sum_{i,k} p_{ik}\Sigma_{ik} \\ q_{mix} = p_0 q_0 + \sum_{i,k} p_{ik} q_{ik} \end{array}\right\}.$$

In this limit we find again that the fluxes $\psi_{ik,cell} \to \psi_{0,cell} \to \psi_{mix,cell}$ where $\psi_{mix,cell}$ is the cell averaged flux one would have obtained for the volume-homogenized region with cross section Σ_{mix} and source q_{mix}.

We have found that in these meaningful limits we have also $r = \Sigma_c/\Sigma \to 1$ and that, therefore, the renormalized treatment of the double heterogeneity in the MOC preserves the natural limits of the stochastic solutions. We investigate now what happens in other limit situations where $r \nrightarrow 1$. To simplify the analysis we consider the case of a matrix with a single type of grain with one layer and analyze the behavior of r in terms of the ratio Σ_1/Σ_0 for p_0 fixed. Figure 1 shows the variation of the ratio Σ/Σ_0 and of $r = \Sigma_c/\Sigma$ with respect to Σ_1/Σ_0.

When the grains are more absorbing than the matrix we have $r = \Sigma_c/\Sigma < 1$ that implies an increase on the transparency of the stochastic region for the renormalized MOC treatment. The opposite, that is, an increase of opaqueness, happens when the matrix is more absorbing than the grains. For MOX fuel the UO_2 matrix is close in total cross section value to the PU_2 grains and therefore $\Sigma_c/\Sigma \sim 1$. In these circumstances the renormalized treatment gives results close to the previous ad-hoc MOC double-heterogeneity treatment.[3] Recall that this previous treatment consisted of setting $\Sigma \to \Sigma_c$ after the calculation of the escape probabilities $\widehat{E}_{ik}$ for the grains and, therefore, $r = 1$. On the other hand, for Gadolinia poisoned PWR fuel or for HTR fuel for which $\Sigma_1/\Sigma_0 > 1$, we have $\Sigma_c/\Sigma < 1$. We examine first the value of the escape probability β. In the ad-hoc MOC method β was calculated with the cross section $\Sigma_c = r\Sigma$ whereas with the renormalized MOC method it is calculated with Σ. Since $\beta(x)$ is a decreasing function of x, we have $\beta_{renorm} < \beta_{adhoc}$ for $r = \Sigma_c/\Sigma < 1$. Since Δ increases with β and $\Sigma\Pi$ decreases with β, the effect is that the renormalized approach increases the effect of the internal sources and decreases the effect of the entering fluxes in the value of the cell-averaged fluxes for the matrix and the layers. At the limit of black grains ($\Sigma_1 \to \infty$) we may neglect the exponential, $\beta(x) \sim 1/x$,

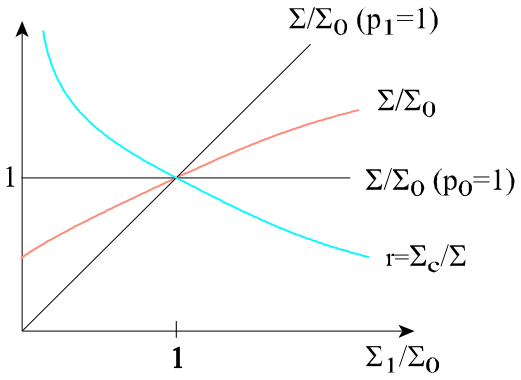

Figure 1: Behavior of Σ/Σ_0 and $r = \Sigma_c/\Sigma$ in terms of Σ_1/Σ_0 for a stochastic mixture matrix-grain. Observe the asymptotic behavior: $r \to \infty$ for $\Sigma_1/\Sigma_0 \to 0$ and $r \to p_0$ for $\Sigma_1/\Sigma_0 \to \infty$. The limiting curves Σ/Σ_0 for $p_0 = 1$ and for $p_1 = 1$ are also indicated.

and we find that, in the absence of internal sources, the transmitted flux is $\psi_+ \sim (1-r)\psi_-$ with $r_{renorm} = \Sigma_c/\Sigma < r_{adhoc} = 1$. For a strong absorber, as Gadolinium, the effect is mainly on the entering fluxes and we may conclude that the renormalized formulation diminishes absorption and increases the transparency of the region.

3 Example calculations

First, we have compared the new renormalized treatment of the double heterogeneity, MOC$_{renorm}$, with the previous one [3] for a set of Kritz experiments.[4] In these experiments, conducted at the Physical Constants Testing Reactor, 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 as in our previous work [3] 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. The results obtained for the experiments without Boron are reported in Table 1. Here and in the following we use MOC$_{adhoc}$ to denote the previous double heterogeneity treatment in the MOC. The first diameter of 0.1 μm is close to the atomic mix limit and both MOC results approach the homogeneous-medium value. Then, as the grain diameter increases so those the difference between the k_∞ values predicted by the MOC$_{adhoc}$ and the new MOC$_{renorm}$ methods.

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 in Table 2 of the linear regression for the k_∞ data 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. Figure 2 shows the regression lines for the experiments, the two MOC methods and the results (not reported here) obtained with the collision probability method using a stochastically homogenized cross section.[3]

Table 1: Comparison of k_∞ MOC results with experimental values for the cases without Boron. All cases have a 2% of PuO2 mass.

$D_g[\mu\text{m}]$	k_∞(experiment)	MOC$_{adhoc}$	MOC$_{renorm}$	$\frac{\text{renorm}}{\text{adhoc}}$-1(pcm)
0.1	1.31467±0.005	1.32303	1.32310	5
52	1.30300±0.005	1.31703	1.31618	-64
107	1.27933±0.005	1.31106	1.30960	-111
195	1.28200±0.005	1.30138	1.29854	-218
328	1.26300±0.005	1.28625	1.28201	-329

Table 2: Linear regression for k_∞ versus grain diameter D for the cases without Boron.

Experiment	MOC$_{adhoc}$	MOC$_{renorm}$
1.3084-14.67 $10^{-5}\times$D	1.3230-11.18 $10^{-5}\times$D	1.3229-12.49 $10^{-5}\times$D

Given the uncertainty in the measured values both slopes, as predicted by the MOC$_{adhoc}$ and the MOC$_{renorm}$ 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.

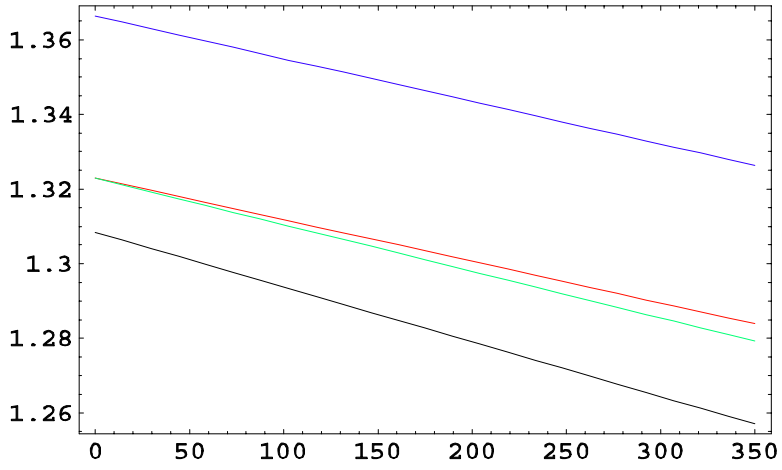

Figure 2: k_∞ versus grain diameter. Lower curve: experiment. Middle curves: characteristic calculations with stochastic solution, lower middle (green) MOC$_{renorm}$, upper middle (red) MOC$_{adhoc}$. Upper curve (blue): collision probability calculations with homogenized cross sections.

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 MOC methods predict sensible values for the k_∞. The two

Table 3: 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}).

$D_g[\mu\text{m}]$	$\rho_{\text{fuel.}}$	PuO_2 mass (%)	Boron	k_∞(exp.)	MOC_{adhoc}	MOC_{renorm}
5×10^{-5}	8.704	2.08	1286±4	0.991	0.97127	0.97126
5×10^{-5}	8.474	2.10	1274±4	0.992	0.97353	0.97354
25	9.540	2.00	1353±4	0.995	0.96404	0.96314
52	8.601	2.29	1350±4	0.992	0.97103	0.97039
107	8.739	2.48	1378±4	0.991	0.98054	0.97905
107	8.638	2.47	1332±4	0.997	0.98552	0.98432
107	7.630	2.45	1227±4	0.989	0.97833	0.97714
195	8.718	2.35	1275±4	0.995	0.97283	0.97070
195	8.657	2.41	1261±4	0.985	0.98128	0.98074
328	8.691	2.42	1163±4	0.992	0.98201	0.97869
328	8.798	2.47	1229±4	0.984	0.97609	0.97270

first rows correspond to the atomic mix limit and both methods give the correct homogeneous-medium result. For all the other cases the new renormalized MOC treatment gives k_∞ values smaller by 100 to 150 pcm than the previous MOC_{adhoc} technique.

Next, we have considered the application of the double-heterogeneity treatment with the MOC to the 2D calculation of an HTGR reactor with prismatic fuel elements.[5] The fuel in this reactor consists of distribution of coated fuel particles embedded in a graphite matrix and requires, therefore, a stochastic treatment. We performed a 99-group, P_0 scattering cross sections, 2D calculation of a BOL core with 1/12 symmetry and a total of 39216 regions. The calculation domain is shown in Fig. 3.

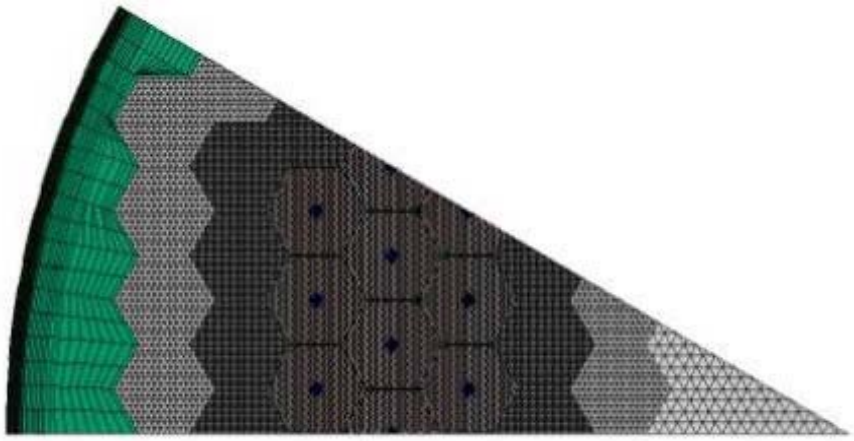

Figure 3: View of the region partition for the 1/12 symmetry HTGR. The central fuel region intersects 10 fuel assemblies.

The calculation was accelerated with the DP_1 synthetic acceleration technique [6] and took under 9 hours in a DEC alpha OSF1 EV7 1Ghz. In Table 4 we compare our results to those obtained

Table 4: Comparisons for the k_{eff} and the ratio production to absorption in the fuel between Monte Carlo and the two MOC calculations. The number between parenthesis are given in pcms (1 pcm=10^{-5}) and correspond to the 1 sigma error interval for the Monte Carlo and to the relative errors, MOC/MC-1, for the MOC results.

	Monte Carlo	MOC$_{adhoc}$	MOC$_{renorm}$
k_{eff}	1.4316 (32)	1.43018 (-99)	1.42881 (-195)
$\frac{production}{absorption}$	1.5753 (45)	1.57662 (84)	1.57644 (73)

Table 5: Normalized assembly fission rates. Comparison MOC - Monte Carlo. The number between parenthesis are given in % and correspond to the 1 sigma error interval for the Monte Carlo and to the relative errors, MOC/MC-1, for the MOC results.

Monte Carlo	MOC$_{adhoc}$	MOC$_{renorm}$
1.004 (0.09)	0.991 (-1.33)	0.997 (-0.76)
0.969 (0.09)	0.959 (-1.12)	0.962 (-0.71)
1.003 (0.09)	0.992 (-1.13)	0.995 (-0.80)
0.916 (0.13)	0.910 (-0.64)	0.912 (-0.39)
0.872 (0.09)	0.871 (-0.11)	0.871 (-0.07)
0.889 (0.09)	0.891 (0.20)	0.890 (0.15)
0.895 (0.13)	0.896 (0.14)	0.895 (0.05)
1.036 (0.12)	1.044 (0.73)	1.041 (0.49)
1.181 (0.08)	1.195 (1.17)	1.189 (0.70)
1.158 (0.09)	1.178 (1.67)	1.171 (1.09)

in [5] by the Monte Carlo method and with the MOC$_{adhoc}$. The new renormalized technique gives slightly smaller values for the k_{eff} and the ratio production/absorption in the fuel domain. In the present case we have a stochastic mixture with appreciably greater cross section in the grain than in the matrix and the analysis of limiting behavior in the previous section predicts an increase in transparency and therefore in leakage. This increase of leakage may explain why the k_{eff} with the new normalized method is smaller than the one for the previous ad-hoc technique.

A more detailed comparison between both double-heterogeneity techniques is given in Table 5 for the integrated fission rates for each one of the 10 fuel assemblies in the geometrical domain. The new renormalized MOC method gives better results, as compared to Monte Carlo, reducing the errors with respect to the Monte Carlo reference by about 40%. Still, as for the MOC$_{adhoc}$ technique, the renormalized method overestimates the power in the inner ring of the core and underestimates it in the outer ring. Note that the MOC$_{renorm}$ values for the assembly power are within 1% of the values predicted by Monte Carlo.

4 Conclusion

In a previous work [3] a stochastic solution for a multicomponent renewal transport process had been developed to calculate mean cell and region fluxes in the method of characteristics for unstructured meshes. Contrarily to the collision probability double-heterogeneity method, this solu-

tion did not require a pre homogenization of the stochastic components. 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 in our previous work an ad-hoc cross section was introduced and used to compute the propagation across the stochastic region.

In this work we have used the cross section predicted by the stochastic solution to compute propagation through the media. Then, to ensure conservation, a factor is applied to the transmission coefficient. Hence, the stochastic solution is fully used throughout and the normalization factor is applied once the transmission has been computed accounting for the stochastic nature of the propagation. As before, an efficient acceleration algorithm has been developed by using the basic assumptions of the DP_N synthetic acceleration previously developed for homogeneous regions.

In contrast with a the treatment previously presented,[3] the new renormalized algorithm preserves the behavior of true stochastic propagation as predicted by the renewal treatment of transport in stochastic media. An analysis of the behavior of the solutions in limiting situations shows that for absorbing grains the renormalized method will increase the transparency of regions containing stochastic mixtures.

A basic difficulty with the validation of the new treatment of the double heterogeneity problem with the MOC is the absence of precise enough experimental data. In this work we have revisited the analysis of the PCTR experiments for the case of non-borated water and compared the renormalized method to the previous one. As before, experimental uncertainties do not allow for a clear decision. But, our results for the cases without Boron allows us to conclude that the renormalized method behaves slightly better than the previous one. As a final example we have used the renomalized method to perform a 2D calculation of a BOL HTGR with a core with a 1/12 symmetry. A similar calculation was done in [5] using the previous MOC treatment and the results were compared to Monte Carlo calculations. We have found that the renormalized MOC method gives still smaller errors in power distribution.

It seems that the renormalized MOC treatment for the double heterogeneity is consistent with the previous formulation, it is more sound theoretically and behaves as good or better in the comparisons with experimental results and Monte Carlo calculations. However, neither one of these is conclusive because there is not enough precision in the experimental results and because the Monte Carlo calculations are not a true reference for a problem with stochastic media. Indeed, Monte Carlo calculations are done for only one possible geometrical configuration of the stochastic components of the problem. However, some confidence can be gained by changing the way used to define the distribution of stochastic components, as was done in [5].

APPENDIX: Synthetic DP_n acceleration

We give here the extension of the DP_N synthetic acceleration to the treatment of the double-heterogeneity MOC formulation. A detailed discussion of the DP_N acceleration is to be found in [8] and technical details on the implementation with the MOC are given in [9].

The DP_N acceleration technique uses a low-order expansion for the cell-averaged angular fluxes and a DP_N angular approximation for the angular fluxes entering and leaving the cells. The latter are taken to be uniform on the cell surfaces. A surface is the common boundary between

two cells or the external boundary of a cell. A similar technique to that used to establish the MOC equations is also applied to the acceleration equations.

We adopt hereon the notation used in [8]. First, a transmission equation is obtained by using (4) to compute the angular moments $\overrightarrow{\psi}_{+,\alpha}$ of the flux leaving through a given surface:

$$A_\alpha \overrightarrow{\psi}_{+,\alpha} = T_{\alpha\beta} \overrightarrow{\psi}_{-,\beta} + V E_\alpha q.$$

Here A_α is a matrix containing moments of the spherical harmonics, $T_{\alpha\beta}$ is the transmission matrix, $E_\alpha = (A_\alpha - \sum_\beta T_{\alpha\beta})/(\Sigma V)$ is the escape probability through surface α, $\overrightarrow{\psi}_{-,\beta}$ are the components of the entering fluxes and q is the stochastic source in (15). The transmission coefficients are given by:

$$T_{\alpha\beta} = \frac{1}{4\pi} \int d\mathbf{\Omega} \overrightarrow{A}_\alpha(\mathbf{\Omega}) \overrightarrow{A}_\beta(\mathbf{\Omega}) \int_{\beta\to\alpha} dS_\perp (1 - r\beta\Sigma), \tag{17}$$

where $\overrightarrow{A}_\alpha(\mathbf{\Omega})$ contains spherical harmonics and the integrations are done over the trajectories entering through surface β to exist via surface α. The main difference with the treatment for the MOC with homogeneous regions is the presence of the factor r in the integrand. Note that for a homogeneous region $r = 1$ and therefore $1 - r\beta\Sigma = \exp[-\Sigma l]$.

Next, a conservation equation is derived by integration on all angular directions and over the cell of the first equation in (13). Multiplying this equation by Σ and integrating in angle and over the cell we get the conservation relation:

$$\Sigma \overrightarrow{\phi}_0 = (B - r^{-1}E)\overrightarrow{Q} + r^{-1}\Sigma S^V \sum_\alpha E_\alpha S^S \overrightarrow{\psi}_{-,\alpha}. \tag{18}$$

In this formula $\overrightarrow{\phi}_0$ and $\overrightarrow{Q}$ are the angular moments of the cell-averaged matrix flux and of the source q, S^V and S^S account for the parity of the spherical harmonics and $E = \sum_\alpha E_\alpha$ is the total escape probability for the cell.

The next step is to eliminate the fluxes and obtain a system of equations for the angular flux moments alone. This is done with Eq. (18). Notice that $q = \Sigma\psi_{as}$ contains external sources and scattering contributions not only for the matrix but also for the grain layers. However, with the help of the second equation in (13), we can eliminate the components corresponding to the layers and obtain an equation for $\overrightarrow{\phi}_0$ in terms of the incoming angular fluxes. Replacing this result in (17) yields the sought system of equations for the surface angular flux moments. A number of techniques have been developed for the fast solution of these equations and we invited the reader to consult [6],[9] for details.

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