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Random Geometry Capability in RMC Code and Applications to Stochastic Media Analysis

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1. Introduction

Fuel design is the key factor to improve the economy and safety of the new nuclear power system, among which the dispersed fuel is one of the most concerned fuel types. Dispersed fuel is the fission fuel grains which are dispersed in the non-fissionable matrices. It has the advantages of fission products containment, high burnup, higher temperature and so on. The dispersed fuel which can be regarded as stochastic media, has been widely used in the Very High Temperature Gas-Cooled Reactors (VHTRs), light water reactors (LWRs) with Fully Ceramic Microencapsulated (FCM) fuel and some experimental research reactors. The delicate transport and burnup calculation is important to the design, analysis and safety of these reactors.

The deterministic methods usually model and calculate stochastic media with approximation such as homogenization to deal with heterogeneity. Special treatment for self-shielding is also needed as the stochastic media has strong effect of spatial and energy self-shielding. Therefore, the deterministic methods have difficulties to meet the requirements in computational accuracy and universality.

On the other hand, Monte Carlo method has advantages on modeling and calculating the stochastic media, due to its precise treatments of complicated geometry and point-wise energy. However, traditional MC codes lacks of the ability to simulate the stochastic media precisely and efficiently. The stochastic media is generally described with the repeated structure, which ignore the random characteristics. Moreover, the cell at boundaries are usually truncated in repeated structures. Burnup calculations of reactors with dispersed fuel is more challengeable for MC codes. The ability to simulate the transport in stochastic media precisely and efficiently is lacked of firstly, and traditional MC codes also lack the ability to handle the massive burnup regions. Even with the above two capacities, special models and methods have to be developed to handle billions of fuel particles in the whole core.

This paper introduces the recently implemented random geometry capability in Reactor Monte Carlo Code RMC [1]. Then the stochastic effects of stochastic media is investigated and analyzed with different random geometry modeling methods. Furthermore, the method of combination of adjacent burnup regions has been proposed and investigated to deal with the burnup simulation of full-core scale.

2. Random Geometry Capability in RMC

Three stochastic geometry modeling methods including Random Lattice Method, Chord Length Sampling and explicit modeling approach with mesh acceleration technique, have been developed in RMC to simulate the particle transport in the dispersed fuels. As have been discussed, Random Lattice Method and Chord Length Sampling are implicit methods with approximations, while explicit modeling approach can reach the best precision with acceptable computational cost when using mesh acceleration technique. In the paper, the Random Lattice Method and explicit modeling approach will be further evaluated and discussed.

2.1 Random Lattice Method

The Random Lattice Method is firstly introduced by MCNP5 [2]. Each time a particle encounters a cell filled by universe flagged as stochastic, a random translation (equation 1) will be performed on the coordinates of the particle. Here, ξ_1, ξ_2 and ξ_3 are independent random numbers in (0, 1). δ_x, δ_y and δ_z are independent maximum displacements in x, y and z directions.

$$\begin{aligned} x &= x + (2\xi_1 - 1) \times \delta_x \\ y &= y + (2\xi_2 - 1) \times \delta_y \\ z &= z + (2\xi_3 - 1) \times \delta_z \end{aligned} \quad (1)$$

2.2 Explicit modeling approach

In the explicit modeling approach, the random packed fuel particles are generated firstly. Then the high-fidelity modeling approach which treats the exact distributions of fuel particles was used to build up the geometry model. Finally, the MC simulation is performed with mesh acceleration technique.

For packing method, Random Sequential Addition (RSA) method [3] is usually used to generate the distributions of fuel particles, which cannot overlap with the boundary and other fuel particles. For modeling approach, a new dispersed-sphere lattice has been developed in RMC. The dispersed-sphere lattice consists of distributed spheres and the gap. The spheres can be filled by universes with detailed structures, supporting Multi-level dispersed-sphere lattices. The mesh acceleration technique is employed for both the generation of distributions of fuel particles or pebbles, and the geometry tracking process. The detailed descriptions can be referred to reference 1.

3. Results and Analysis of Stochastic Effect

The Random Lattice Method and explicit modeling approach were evaluated, and the stochastic effects were investigated.

3.1 Evaluation of Random Lattice Method

The typical TRISO fuel is used, of which the dimensions are listed in Table. I. The TRISO fuel has 5 layers, and in the 5×5×5 regular lattice the lattice pitch (L) is 0.1982 cm, as is shown in Fig. 1. The reflective boundaries are used for the outer boundaries.

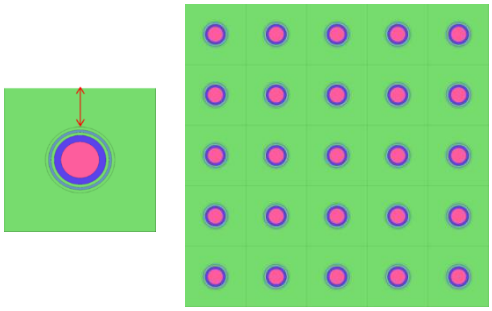


Fig. 1 TRISO fuel and regular lattice of TRISO fuels

Table. I Dimensions and components of TRISO fuel

Layer	Radius/cm	Density/ g/cm^3	Material
Layer 1	0.025	10.4	UO_2
Layer 2	0.034	1.1	C+^{10}B+^{11}B
Layer 3	0.038	1.9	C+^{10}B+^{11}B
Layer 4	0.0415	3.18	SiC
Layer 5	0.0455	1.9	SiC
Outside		1.9	C+^{10}B+^{11}B

Table. II Kinf with different numbers of lattices

	RMC	MCNP	Delta
Regular lattice	1.58593	1.58604	-0.00011
3×3×3	1.588157	1.58799	0.000167
5×5×5	1.587974	1.58814	-0.00017
101×101×101	1.587866	1.58732	0.000546

The random translations are applied to the regular lattice model with random disturbance, i.e. δ in equation 1. Here, δ=L/2-r is the largest disturbance, where L is the lattice pitch and r is the radius of the TRISO fuel. 10000 neutrons are used for totally 1500 cycle with 500 inactive cycle, leading to the standard deviation of 0.0002 on Kinf. The URAN card in MCNP5 is used for reference. The results of Kinf with different numbers of lattices are shown in Table. II. Here, the discrepancies are equal to Kinf of RMC minus Kinf of MCNP. It can be found that the discrepancies between RMC and MCNP for four cases are close to the standard deviation. The discrepancy of RMC between 3×3×3 and 5×5×5 is 0.000183, and -0.000108 between 101×101×101 and 5×5×5. It can be concluded that the Kinf of random lattice method is not related to the numbers of lattices. It means that the effects due to random distributions will not vanish or decrease when the system grows larger.

3.2 Stochastic effects of explicit modeling

The random distributions of the TRISO fuel are generated by RMC. In Fig. 2, the packing faction is 0.05068 in the dimensions of the 5×5×5 pitches. 10000 neutrons are used for totally 1500 cycles with 500 inactive cycles, resulting in the standard deviation of 0.0002 on Kinf. 40 different realizations have been created by 40 different random number sequences. The statistics results of Kinfs are shown in Table. III and Fig. 3.

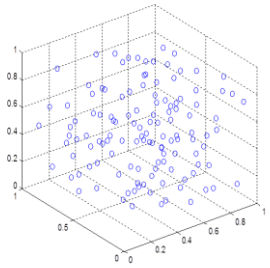


Fig. 2 Random distributions of the TRISO fuel

Table. III Statistics results of Kinfs

Ave	1.589337
Min	1.588732
Max	1.590011
Max-Min	0.001279
SD	0.000296

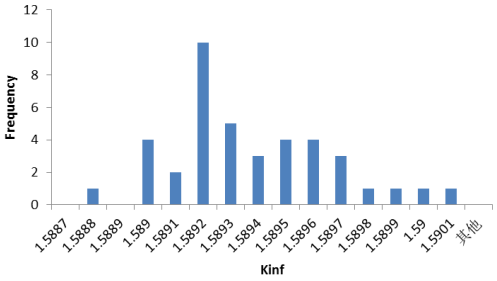


Fig. 3 Distribution of Kinfs

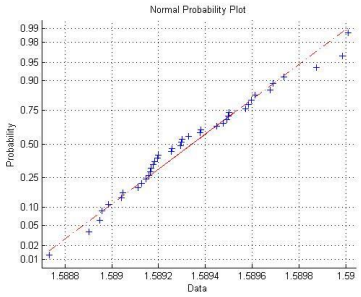


Fig. 4 Normality tests for 40 observations

It can be found that the distribution of Kinfs seems like a normal distribution whose average is 1.589337 and standard deviation is 0.000296. The normality tests for the 40 observations were carried out by the "normplot" function of MATLAB, as shown in Fig. 4. It shows that the 40 observations obey the normal distribution.

The maximum difference is 127.9 pcm (0.001279). The standard deviation of distribution is close to the statistical deviation of RMC (0.0002). It means that when the number of particles and the packing faction are large, the result of a single realization approaches the averaged value. The averaged Kinf which is regarded as reference is 340.7 pcm larger than that of lattice model, and 136.3 pcm larger than random lattice model.

4. Burnup Calculations of Stochastic Media

The problem of memory footprint is inescapable when the burnup calculations are carried on for ten millions or a hundred millions random distributed fuel particles. If each TRISO particle is regarded as an individual burnup region, the memory footprint would be unacceptable. Therefore, the method of combination of adjacent burnup regions is hereby proposed and investigated.

The procedures of combination of adjacent burnup regions are described as followed:

1. A framework of virtual Cartesian meshes is introduced to the area filled with TRISO particles, which divides the TRISO particles into different groups, as shown in Fig.5. The particles belong to those meshes in which their centers are located. Each of this group consisting of adjacent TRISO particles is regarded as the same burnup region. For example, particles 1, 2, 6 are regarded as a combined burnup region, while particles 7, 8, 9 are regarded as another combined burnup region;
2. If there are several types of fuel particles inside one mesh, those different fuel types are treated as different burnup regions. For example, in Fig.12 particles 1, 2, 6 are regarded as a combined burnup region, while particles 3, 4, 5 are regarded as another one. This treatment make it possible to deal with burnup when different types of particles are mixed together, such as fuel particles and poison particles;
3. Then the burnable cells in the lowest level of the hierarchy geometry are automatically expanded in the dispersed-sphere lattice structure. The burnable cells are expanded according to the partition of combined burnup regions defined above;
4. The mass of fuel particles are added within the same burnup region when the mass of the burnup region is calculated;
5. Due to the combination of burnup regions, the geometrical cells are no longer matched with the burnup regions one by one (which used to be matched one by one before the combination). Therefore, the geometrical cells are mapped with the combined burnup regions.
6. The geometrical cells will converted to the combined burnup regions during the transport process, so as to tally the isotopic cross sections and flux in the burnup regions.

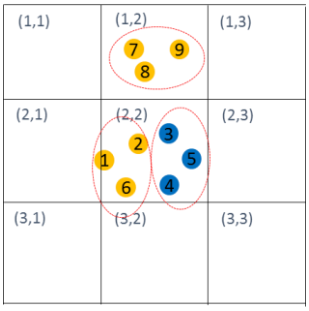


Fig. 5 Combination of burnup regions based on virtual meshes

The model of prismatic super-cell [4] with 3000 TRISO fuel is used, as is shown in Fig. 6. The super-cell is 49.3 cm height, with void boundary at one end in the axial direction, while reflective boundary at other five faces, as shown in Fig. 7. In order to reduce the memory footprint, it is effective to divide fuel particles into several regions, and combine particles in the same region. Before combining, the number of regions must be decided. Therefore, the axial flux distribution is firstly calculated. However, instead of the detailed geometry with dispersed particles, the volume-mixed atomic nuclides densities are used in the fuel region to save the calculation time.

For the flux tally, there are 1000 bins in axial direction, and two groups of fluxes are tallied, whose energy boundary is 0.625eV. The fast fluxes of atomic-mixed model and 3000 particles model are normalized and compared in Fig. 8. It can be found that the trends are almost the same for atomic-mixed and detailed model. The thermal, fast and total fluxes are compared in Fig. 9, showing that the trends of two groups are also similar. Judging from the gradient of trend, 40 axial burnup meshes is suitable, as is shown in Fig. 8.

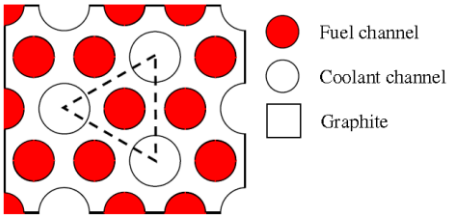
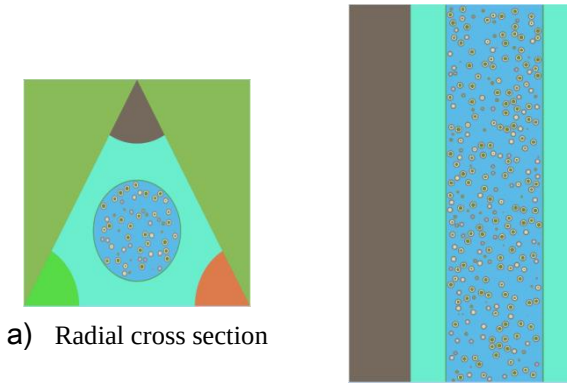


Fig. 6 Infinite lattice of fuel and coolant channels



a) Radial cross section

b) Axial cross section

Fig. 7 Explicit modeling of prismatic super-cell

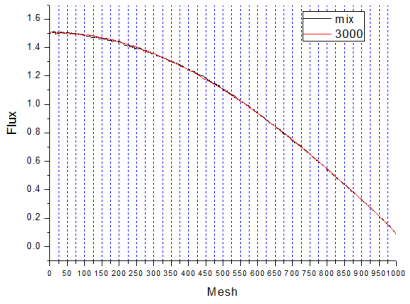


Fig. 8 Fast fluxes of atomic-mixed and detailed model

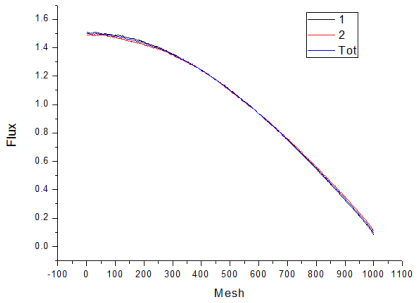


Fig. 9 Two groups fluxes

The memory footprints of 1, 40 and 3000 burnup regions at different burnup step are shown in Table. IV. It can be found the memory saving is significant, in which the memory saving of 40 regions and one region are close. Kinf evolution of different burnup regions number is shown in Fig. 10. It can be found that Kinf of 40 regions are close to 3000 regions, while the discrepancies between one and 3000 regions are larger. Therefore, with the void boundary, reasonable and adequate burnup regions are necessary to maintain the computational accuracy. Moreover, as the memory saving of 40 regions is close to that of one region, 40 regions are adequate to maintain the computational accuracy and effective for memory saving.

Table. IV Memory footprint of different burnup regions

Burnup (MWD/KgHM)	Memory/kb			Delta40-3000/%	Delta1-3000/%
	3000	40	1		
0	160004	48064	44988	-69.96	-71.88
0.1	190508	67464	65144	-64.59	-65.81
0.5	247336	92168	99100	-62.74	-59.93
1	271236	121724	124000	-55.12	-54.28
2	297164	148448	135980	-50.05	-54.24
3	329644	162936	158548	-50.57	-51.90
4	358112	177576	179896	-50.41	-49.77
5	380184	185248	198568	-51.27	-47.77
6	396360	197132	207652	-50.26	-47.61

Table. V Calculations time of different burnup regions

Burnup (MWD/KgHM)	Time/Min			Delta40-3000/%	Delta1-3000/%
	3000	40	1		
0	4.3866	3.4881	3.4390	-20.4828	-21.6022
3	33.3923	22.1624	21.7254	-33.6302	-34.9389
6	52.7422	34.7798	33.9980	-34.0570	-35.5393

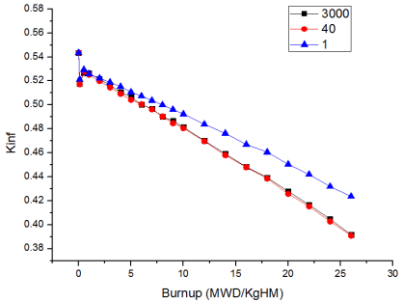


Fig. 10 Kinf evolution of different burnup regions number

The calculations time of different burnup regions are also shown in Table. V. Both the calculations time of 40 regions and one region are reduced compared with 3000 regions. Moreover, calculations time of 40 regions is slightly more than one region, which means that 40 regions is reasonable in term of time consuming.

5. Conclusions

In this paper, the newly developed random lattice method and explicit modeling method of RMC were introduced and applied to investigate the stochastic effect of stochastic media. Results show that Kinf of random lattice method is not related to the numbers of lattices. It means that the difference between repeated lattice and random geometry will not vanish or decrease when the system grows lager.

For explicit modeling method, when the number of particles and the packing faction are large, the result of a single realization approaches the averaged value. The averaged Kinf regarded as reference is 340.7 pcm larger than that of lattice model, and 136.3 pcm larger than random lattice model.

The method of combination of adjacent burnup

regions has been proposed and investigated. Results show that with reasonable and adequate burnup regions, this method can effectively reduce the memory footprint while keeping the computational accuracy. The method of adjacent burnup regions combination can be easily extended to the burnup simulation of full-core scale in the future research.

Acknowledgements

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