Modeling and Simulation of Dispersion Particle Fuels in Monte Carlo Neutron Transport Calculation

CHEN Zhenping，XIE Jinsen，GUO Qian，XIE Qin，YU Tao*

University of South China, Hengyang, Hunan 421001, China

Abstract: The dispersion particle fuel has advantages of high burnup, strong ability of containing fission products and good thermal conductivity. It is widely used as an advanced fuel element in next-generation nuclear reactors, such as the Molten Salt Reactor and High Temperature Gas Cooled Reactor. However, the dispersion fuel element in which the fuel particles randomly distributed in the matrix material presents new challenges for the conventional reactor physics methods. Based on the Monte Carlo method, the sub-fine lattice method for modeling of dispersion particle fuels in neutron transport simulation was studied, and the impacts on the modeling efficiency and calculation accuracy of the lattice grid sizes were given. The numerical results showed that the sub-fine lattice modeling with optimal lattice size can meet the requirements of reactor physics simulations for the dispersion particle fuel.

Keywords: Monte Carlo, particle fuel, sub-fine lattice model, reactor physics

1. Introduction

In order to promote the safe, efficient and sustainable development of nuclear energy, the world is stepping up efforts to develop the fourth generation nuclear energy system with better safety and economy. The Dispersion Particle Fuels (DPF) has been widely used in High Temperature Gas-cooled Reactor (HTGR) [1] and Solid Molten Salt Reactor (SMSR) [2], and in conceptual design of the new type of Pressurized Water Reactor (PWR) [3], because of its deep burnup fuel consumption, inclusive of fission product capability and good thermal conductivity. Because of the random distribution of fuel particles in matrix materials, the dispersion particle fuels bring great challenges to the traditional reactor physics calculation methods. The traditional "two step method" can not fully meet the requirements of current reactor physics calculations [4], especially for the complex models filled with various types of fuel particles (such as burnable poison particles). Therefore, the random distribution characteristics of the fuel particles should be fully considered in order to obtain the reliable reactor physics simulation results. This paper focuses on using the Monte Carlo method to simulate the neutron transport in the dispersion fuel models. The basic principle and method of constructing stochastic model for fuel particle using the Sub-Fine Lattice (SFL) method was presented. Furthermore, the influence of lattice sizes on the stochastic modeling efficiency and reactor physics calculation precision was discussed.

2. Dispersion Particle Fuels (DPF)

Dispersion Particle Fuel [5] is an advanced form of nuclear fuel element, which is composed of fuel particles (U or Pu compound) homogeneously distributed in the inert matrix materials (such as metal, ceramic or graphite and other non fissile

*Corresponding author: yutao29@sina.com

materials). The dispersion particle fuel is mainly used in the core design of high temperature gas cooled reactor and solid molten salt reactor.

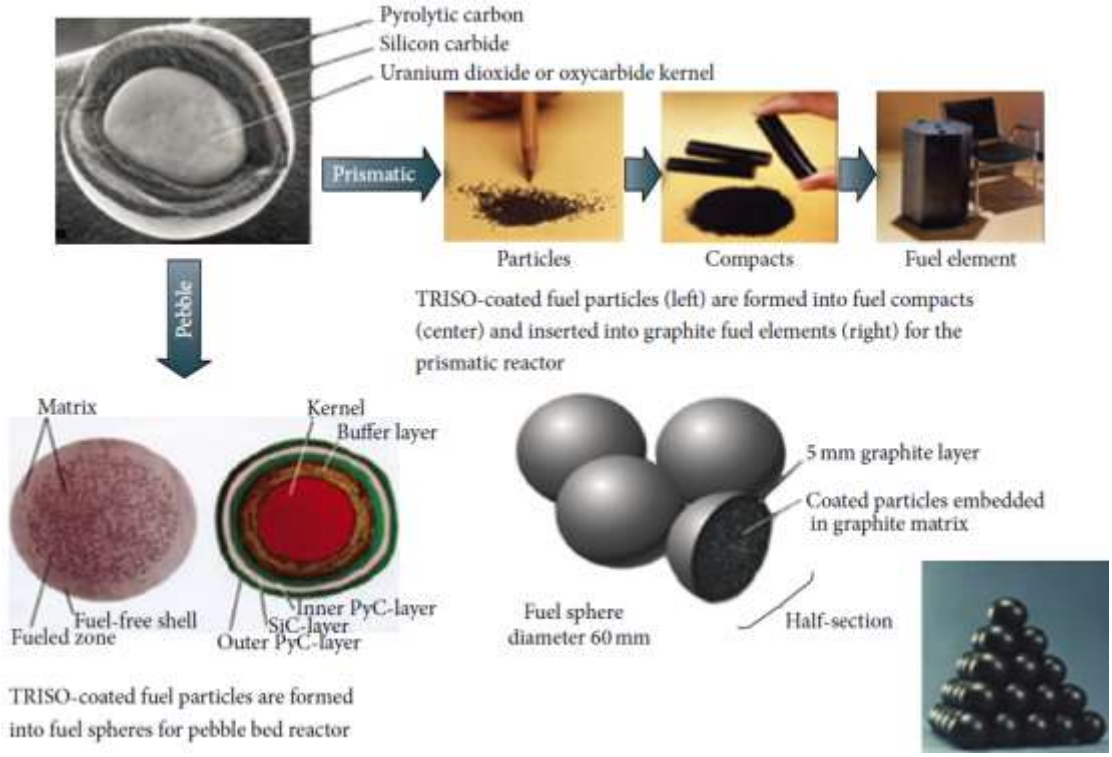


Figure 1. TRISO-type dispersion particle fuels for HTGR

In the fourth generation nuclear power system, the spherical fuel element is usually used in the pebble bed reactor, and the fuel particle is dispersed randomly in the graphite matrix. The pebble bed reactor core will be loaded with a certain amount of spherical fuel element (fuel pebble) into the reactor core. Taking the traditional HTGR [6] as an example, each fuel pebble consists of a spherical fuel zone with radius 2.5cm and an outer graphite shell with thickness 0.5cm. In the fuel pebbles, the most important component is the TRISO (Trstructural ISOtropic) type coated fuel particles (Figure 1) [7]. The TRISO fuel particles, up to about 1mm in diameter, consist of a fuel kernel and four coating layers which prevent the leakage of fission products and provide structural integrity. These fuel particles are randomly distributed in the fuel pebble for the pebble-bed design or in the fuel compact for the prismatic design.

In DPF nuclear systems, the randomly distributed fuel particles represent effective point absorbers for resonance energy neutrons, combining with the usual fuel rod or fuel pebble heterogeneity to yield the "double heterogeneity" for particle fuel. The irregular distribution of fuel particles in fuel elements is caused by the processing and manufacturing of fuel elements. In the manufacturing process, the distribution of the fuel particles in the element can not be artificially setted, which is usually difficult to achieve in the manufacturing process of the fuel elements. This is the main reason leading to the random distribution of fuel particles in the fuel element. Thus, the dispersion particle fuels bring great challenges to the traditional reactor physics calculation methods. Special care must be taken to analyze this fuel in order

to predict the spatial and spectral dependence of the neutron population in a steady-state reactor configuration. The essential challenge consists in developing a methodology that can accurately and efficiently analyze the double heterogeneity configuration and predict the eutronic properties at both the microscopic and macroscopic levels in the global neutronic computation, as well as accounting for the nature of the stochastic distribution in the DPF reactor design. Thus, it is necessary to carry out studies on stochastic modeling and neutron transport calculation method for dispersed particle fuels.

3. Sub-Fine Lattice (SFL) Stochastic Modeling

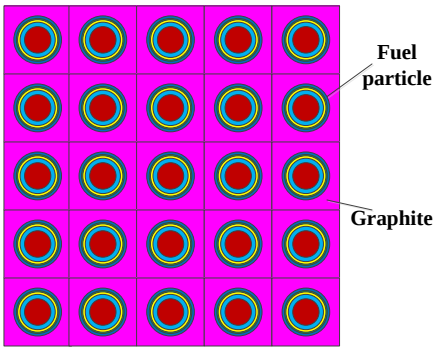


Figure 2. Lattice modeling for DPF fuels

Lattice model is one of the most commonly used methods for DPF fuels modeling [8]. As shown in Figure 2, a series of regularly distributed lattice grids are constructed, and each fuel particle is placed at the center of the lattice grid. Generally speaking, in order to ensure the modeling efficiency, the lattice size of the traditional lattice model is much bigger than the fuel particle size, and each lattice contains only one fuel particle. The biggest drawback of the traditional method is difficult to maintain the required fuel volume packing fraction (usually less than 0.524). As a result, it is difficult to be applied in engineering application [9]. At the same time, the traditional lattice model can not consider the random distribution of fuel particles in the graphite matrix, so the effective multiplication factor in the assembly calculation results in an error 0.1%~0.2%[10], and greater errors will be produced for the whole core calculations.

The Sub-Fine Lattice [11] model is a random distribution model, which is further developed from the traditional lattice model. Compared with the traditional lattice model, the sub-fine lattice model also uses the regular distributed lattice grid to place the fuel particles, but the central point of the fuel particles are randomly distributed in the lattice grid. Therefore, the sub-fine lattice model is a stochastic model which takes into account the stochastic distribution of fuel particles in the graphite matrix. In the modeling of the sub-fine lattice model, the size of the lattice grid is not needed to be strictly specified. However, some previous study [12] indicated that the lattice grid with a size of $2R/\sqrt{3}$ (i.e. R is the radius of the fuel particle) will be a good choice to guarantee that each lattice can contain only one particle center point and to improve the modeling efficiency. Therefore, the basic principle and implementation procedure of the sub-fine lattice model are as followling (Figure 3):

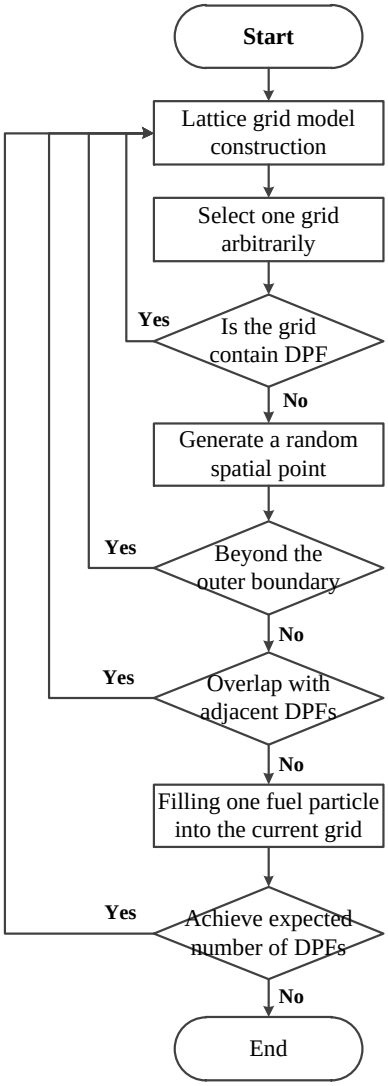


Figure 3. The modeling scheme of sub-fine lattice model for DPF

(1) According to the given lattice grid sizes, a three-dimensional lattice grid model with regular distribution is established;

(2) A lattice grid is selected randomly, and then determining whether the selected grid is filled with fuel particle or not;

(3) If the selected lattice grid has been filled with fuel particles, return to step (2); otherwise, enter into step (4);

(4) In the selected lattice grid, a spatial point will be generated randomly using the sampled pseudo random number, and the center of the fuel particle will be placed at that point;

(5) Check whether the fuel particle beyond the outer boundary of the model; if it's ture, return to step (2), otherwise go forward into step (6);

(6) Check whether the fuel particle in the current lattice grid overlap with the fuel particles located in the adjacent lattice grids; if it's true, return to step (2), otherwise enter into step (7);

(7) A fuel particle is placed at the generated spatial point in the current selected lattice grid;

(8) Determine whether the fuel particles filled in the model achieve the expected number, or whether the volume packing fraction of the fuel particles reaches the expected value; if not, return to step (2); otherwise, the modeling will be established.

The sub-fine lattice model usually chooses smaller lattice grid size than the traditional lattice model, and allows the center point of the fuel particles to be placed randomly. Therefore, compared with the traditional lattice model, the sub-fine lattice model can maintain the required fuel packing fraction in the practical applications. Furthermore, the model considers the random distribution characteristics of fuel particles in the graphite matrix, which is more consistent with the needs in practical engineering applications.

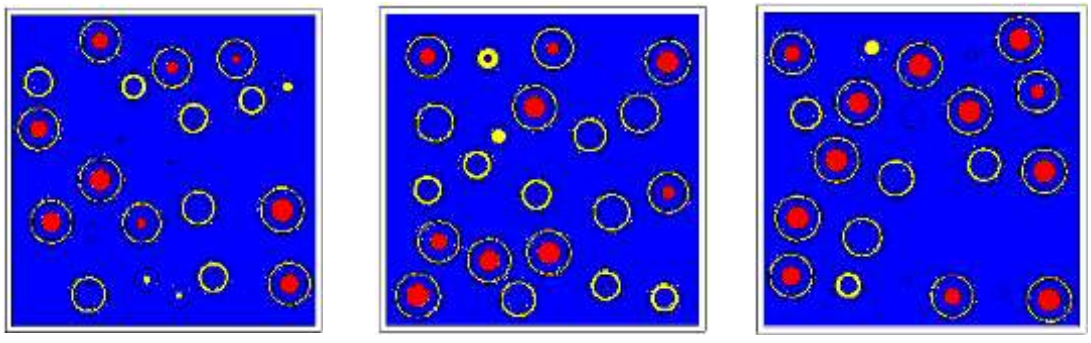
4. Numerical Results and Analysis

4.1 Sub-Fine Lattice (SFL) Model Numerical Verification

In order to verify the correctness and reliability of the sub-fine lattice method and the development procedure, a self-developed TRISO particle fuel model was used for numerical verification. A graphite matrix cube model with a side length of 0.4754 cm was defined, and 100 TRISO coated fuel particles were randomly filled in the model based on the Sub-Fine Lattice (SFL) method. The specific materials, dimensions and specific geometries of the TRISO fuel particles used in the model are taken from the NGNP high temperature gas reactor design [13].

Table 1. TRISO Fuel kernel geometry and composition

Material	Thickness (μm)	Nuclide composition	Density (g/cm^3)
Uranium oxycarbide	175	$UC^{0.5}O^{1.5}$	10.5
Porous carbon buffer	100	C	1.0
Inner pyrolytic carbon	40	C	1.9
Silicon carbide	35	SiC	3.2
Outer pyrolytic carbon	40	C	1.9



(a) X-Y cross-sectional view (b) Y-Z cross-sectional view (c) X-Z cross-sectional view

Figure 4. The cross-sectional views of the model

In the defined model, the graphite matrix used is H-451 type graphite which is commonly used in the American prism type high-temperature gas cooled reactor. The density is set to be $2.25 g/cm^3$. In this model, uranium fuel is used with low enrichment of uranium carbide and uranium dioxide, in which the enrichment of

uranium-235 is 10.36% and the atomic ratio of U, C and O is 2: 1: 3. The different view sections of the model constructed with lattice grid size of $2R/\sqrt{3}$ are shown in Figure 4. It can be seen from the figures that the TRISO fuel particles in the graphite matrix has a good random distribution characteristics.

The Monte Carlo particle transport calculation program MCNP developed by the Los Alamos National Laboratory was used to calculate the Infinite proliferation factor (k_∞) for the custom model. In the MCNP calculation, the boundary conditions for the outer boundary of the model were set to be reflective boundary conditions. The Monte Carlo critical simulation for the model was performed with 300 inactive and 700 active criticality cycles of 1000 source neutrons. The result of Random Sequential Addition (RSA) was taken as a reference. It can be seen from Table 2 that the error of the sub-fine lattice method is 0.16%, which is consistent with the reference value of the RSA method. The numerical results indicate the correctness of the sub-fine lattice method and the modeling procedures.

Table 2. Sub-Fine Lattice (SFL) model numerical verification

Modeling method	k_∞	Statistical error(σ)
SFL method	1.29265	0.00087
RSA method	1.29058	0.00095

4.2 Analysis of the Sub-Fine Lattice Grid Size

In order to analyze the effect of sub-fine lattice grid sizes on modeling efficiency and computational accuracy for dispersion fuel particle model, the influence of grid sizes is studied in this section. Firstly, the influence of sub-fine lattice grid sizes on the modeling efficiency of the dispersion fuel model is studied. The testing model is same with the model used in section 3.1, namely the graphite cube model with a side length of 0.4754 cm. The modeling efficiency was analyzed when filling different amounts of fuel particles into the model with different grid sizes of the sub-fine lattice model.

Table 3 Modeling efficiency when the sub-fine lattice size is $2R/\sqrt{3}$

Number of fuel particles	Modeling time (s)
10	0.101
45	0.589
75	1.741
100	7.908

Table 4 Modeling efficiency when the sub-fine lattice size is R

Number of fuel particles	Modeling time (s)
10	0.097
45	0.568
75	1.507
100	7.250

Table 5 Modeling efficiency when the sub-fine lattice size is $2R/\sqrt{5}$

Number of fuel particles	Modeling time (s)
10	0.244
45	1.342
75	4.695
100	25.540

Table 3 to Table 5 shows the numerical relationships between the modeling efficiency with the sub-fine lattice grid sizes. From the Table 2 and Table 3, we can see that when the number of fuel particles is large, the modeling time of with grid size of R is slightly smaller than that of modeling with grid size of $2R/\sqrt{3}$. This is the fact that the number of lattice grids with grid size of R is slightly more than that of with grid size of $2R/\sqrt{3}$, and the sampling speed is slightly faster. At the same time, it can be seen from Table 5 that the modeling with grid size of $2R/\sqrt{5}$ spends much more time than those of modeling with grid size of R and $2R/\sqrt{3}$. The main reason is that when $2R/\sqrt{5}$ is used as the grid size, the number of lattice grids that need to be overlapping checked will be the 342 grids around the center grid (currently filled grid), rather than the first two case of 124 grids. This is about 2.76 times slower than that of the first two cases. So the modeling with the grid size of $2R/\sqrt{5}$, the number of overlap checking is large, and the corresponding modeling speed will be much slower. It's about three times as long as the first two cases. The time will continue to increase when the smaller grid size is used or more number of fuel particles is filled. Now we can conclude that, from the viewpoint of modeling efficiency, the best size of the lattice grid is R, and the secondary is $2R/\sqrt{3}$; if not necessary, try not to select $2R/\sqrt{5}$ or smaller grid sizes, which will make the modeling time increase rapidly.

In order to further test the effect of different grid sizes on the accuracy of Monte Carlo neutron transport calculations, the model of Section 3.1 is carried out by using grid sizes of $2R/\sqrt{3}$, R, $2R/\sqrt{5}$. Then the infinite multiplication factor (k_∞) was calculated using the MCNP program. The result of RSA model is used as the reference value. The influence of different grid sizes on the calculation accuracy would be analyzed.

Table 6 Effects of different grid sizes on calculation accuracy

Grid size	k_∞	Statistical error (σ)
$2R/\sqrt{3}$	1.29265	0.00087
R	1.29134	0.00087
$2R/\sqrt{5}$	1.29032	0.00091
RSA	1.29058	0.00095

The effects of different lattice grid sizes on calculation accuracy were given in Table 6. It can be seen from the table that the k_∞ value calculated by the MCNP program based on the stochastic model of the sub-fine lattice decreases with the decrease of the grid size, and is close to the reference value of the RSA model. Obviously, it can introduce a greater randomness for the model, which is closer to the

true distribution of fuel particles. Because the number of locations that can arrange the the fuel particles increases as the lattice grid size decreases, and the area where the fuel particles can be reached increases. At the same time, as the lattice grid size decreases, the number of grids that need to be overlapping checked during modeling will increase and then the modeling speed will become slower. Theoretically, when the lattice grid size tends to be zero, the number of grid need to be overlapping checked will also tend to be infinity. Under this situation, the sub-fine lattice model has actually been transformed into the RSA model. Thus, as the lattice grid size decreases, the sub-fine lattice model will tend to be the RSA model. When the lattice grid size is equal to zero, actually, the sub-fine lattice model has become RSA model.

4.3 Discussion and Analysis

From the numerical results shown in section 3.1 and 3.2, the following conclusions can be concluded. With the lattice grid sizes decreasing, the sub-fine lattice model will tend to be the RSA model, which will increase the randomness of the sub-fine lattice model. Meanwhile, the decreasing in lattice grid sizes will lead to a rapid increase in modeling time, which makes the sub-fine lattice model lose its greatest advantage on modeling efficiency. Therefore, it is necessary to select the appropriate grid size to balance the modeling efficiency and calculation accuracy according to the specific situations. When modeling efficiency is primarily considered, there is need to select a larger lattice grid size for modeling. If the calculation accuracy is primarily considered, the grid needs to be chosen with smaller sizes. So the randomness of the sub-fine lattice model with a grid size of R is larger than that of the model modeled with a grid size of $2R/\sqrt{3}$, and the modeling speed with a grid size of R is faster than that of the model with a grid size of $2R/\sqrt{5}$. Therefore, to balance the modeling efficiency and calculation accuracy, it is recommended to use the grid size of R as the optimal grid size to perform the DPF fuels modeling.

5. Conclusion

The random distribution of dispersion particle fuels brings great challenges to the traditional reactor physics calculation methods. Based on the Monte Carlo neutron transport method, the basic principle and implementation scheme of sub-fine lattice model for stochastically modeling the dispersion particle fuels were presented. The modeling efficiency and calculation accuracy of the sub-fine lattice model were tested and verified using the TRISO-type particle fuel models. It can be seen from the numerical results that the calculation results of the sub-fine lattice model are in good agreement with the reference results, which demonstrates the effectiveness and correctness of the modeling method. Meanwhile, the lattice grid size used in the sub-fine lattice model will have a great influence on the modeling efficiency and the calculation accuracy. To balance the efficiency and accuracy, it is recommended to use a grid size of R as the optimal size in DPF modeling and simulation.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (No. 11605085, No. 11575079), the Scientific Research Fund of Hunan Provincial

Education Department of China (No. 16B222, No. 16C1361), and the Scientific Research Found of University of South China (No. 2015XQD06, No. 2015XQD12). And the authors would like to show their great appreciations to NEAL (Nuclear Engineering and Application Laboratory) Team for its contribution to this research.

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