Proceedings of the Reactor Physics Asia 2015 (RPHA15) Conference
Jeju, Korea, Sept. 16-18, 2015

Development of New Statistical Geometry Model using the Delta-tracking Method

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1. Introduction

In the case of neutron transport calculations for typical reactors such as light water reactors or fast breeder reactors, the spatial positions of nuclear fuels are usually known. However, in the case of coated fuel particles in the fuel compact used in very high temperature reactor (VHTR), we should treat a more complicated geometry where fuel particles are randomly distributed in the system. In order to calculate such stochastic geometry using the Monte Carlo method, the statistical geometry model (STGM) has been developed and implemented in the existing Monte Carlo codes [1,2].

In the accident of Fukushima Daiichi Nuclear Power Station, the meltdown of core results in the formation of corium, thus we should expect variety of fuel debris forms in various moderating conditions. Consequently, there are large uncertainties, e.g., the distribution of fuel debris in the system. As one of the possibilities, fuel debris could be randomly distributed in water. It is difficult to rigorously analyze neutronics characteristics for such random geometry, while these random geometry can be effectively treated by the STGM. However, in using STGM, there are some implicit limitations such as fuel particle radius. The applicability and validity of STGM has not been sufficiently discussed. In the present study, we propose a new STGM algorithm using the delta-tracking method to cope the limitation of the traditional STGM model.

2. Delta-Tracking Method

During the random walk of neutron, it is necessary to analysis the neutron collision points. Generally, analysis of collision points is carried out as follows:

1. Search the intersection point of neutron flight path and boundary of nearest neighbor area.
2. Calculate the neutron flight length.
3. Move the neutron to the next boundary area, if the flight length goes over the intersection point of boundary area.
4. The intersection point is assumed as the new emitting point, and then iterate the procedures from 1 to 3.

However, longer calculation time is necessary for flight analysis as the complexity of geometries become increases, such as random distribution of fuel particles in three dimensional geometry.

So, in order to increase computational efficiency of flight analysis, we introduced the delta-tracking method [3,4]. Delta scattering is a non-physical scattering reaction by which energy and flight direction of neutron do not change. Magnitude of the delta scattering cross section can be set arbitrary. Total cross sections including delta scattering are set to be spatially constant throughout the geometry as follows:

$$\Sigma_{t,g}^{*} = \Sigma_{t,g}(\vec{r}) + \Sigma_{s,g}^{*}(\vec{r}) \qquad (1)$$

$\Sigma_{t,g}^{*}$ is a total cross section involving delta scattering in energy group g, $\Sigma_{t,g}(\vec{r})$ is a total cross section in position $\vec{r}$ and energy group g, $\Sigma_{s,g}^{*}(\vec{r})$ is a delta scattering cross section in position $\vec{r}$ and energy group g.

$\Sigma_{t,g}^{*}$ is usually set to the maximum value of total cross section throughout the system in the given energy group. By using $\Sigma_{t,g}^{*}$, total cross section becomes a constant value throughout the system and thus the system can be considered as a homogenized single area such as Fig. 1 from the viewpoint of flight analysis. Consequently, flight analysis can be faster. With the delta-tracking method, flight analysis algorithm of random walk is simplified as follows:

1. Determine the neutron source.
2. Sample the neutron flight length using $\Sigma_{t,g}^{*}$.
3. Determine the material at reaction point.

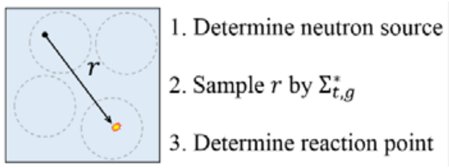

Fig. 1. Determination of collision point utilizing the delta-tracking method.

3. Proposal of New Calculation Model for STGM

On the current STGM model, delta scattering is not used for neutron flight analysis. In the current STGM method, outgoing point of a neutron from a fuel particle is determined at first, then the distance to the nearest fuel particle is sampled by the nearest neighbor distribution (NND), which is the probability distribution of distance between fuel particles. In a fuel particle, ordinary flight analysis is carried out. The advantage of this model is as follows; positions of all of fuel particles are not necessary in advance and collision estimations with these fuel particles are not necessary during flight analysis [1].

On the other hand, all regions are virtually “homogenized” thus outgoing point of a neutron from a fuel particle is not explicitly determined. In such algorithm, direct application of the current STGM method is difficult since the outgoing point of a neutron is not known, thus the nearest neighbor distribution cannot be used. Furthermore, overlapping of fuel particles, which is not physically allowed, is implicitly assumed in the estimation of NND. Consequently, calculation accuracy becomes worse as the fuel particle radius becomes large, as shown in Fig. 2[5]. In this section, we propose a new STGM algorithm using the delta-tracking method.

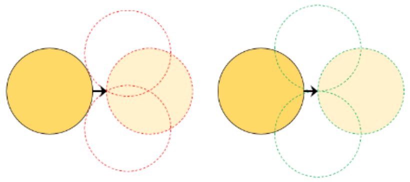

Fig. 2. Interference effect between two fuel spheres: overlapping of fuel particles is implicitly assumed

3.1 Random walk algorithm

In the delta-tracking method, the materials at neutron generation collision points are necessary for flight analysis. In the common delta-tracking calculation, these information is easily known since material spatial distribution is known. However, in the STGM we can sample the material of initial neutron source by using the average packing fraction but not know the explicit material distribution in advance. In order to resolve this issues, the following approaches are used.

3.1.1 Material Assignment at Collision Position

In the average sense, packing fraction can be assumed spatially uniform throughout the calculation system. When the packing fraction is assumed to be spatially uniform, material assignment at collision position is easy, i.e., material (fuel particle or moderator) can be statistically assigned according the packing fraction. However, in reality, the packing fraction has spatial distribution especially the neighbor region of a fuel particle. When many fuel particles with finite radius are randomly distributed, these fuel particles may have physical contact and it causes local fluctuation of the packing fraction near a fuel particle. Thus in the application of STGM this fluctuation should be taken into account.

In order to appropriately treat the fluctuation of the packing fraction, we introduce a radial distribution function of the packing fraction $f_p(r)$. $f_p(r)$ is defined as a volume ratio of fuel to total (fuel + moderator) at distance r. Thus, by using a uniform random number ξ from 0 to 1, it is able to decide material at the collision point as follows:

- $\xi > f_p(r)$: material at collision point is moderator,
- $\xi < f_p(r)$: material at collision point is fuel.

In the present improved model, two different radial distribution functions are necessary depending on the type of neutron generation point as shown in Fig. 3.

- $f_{p1}(r)$: neutron source point is in a fuel particle.
- $f_{p2}(r)$: neutron source point is in moderator.

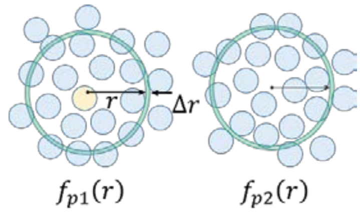

Fig. 3. Radial distribution function of packing fraction.

3.1.2 New STGM Algorithm

The random walk algorithm of neutron using the new STGM algorithm is as follows (Fig.4):

1. Determine a material of the starting point. The starting point on the first batch is decided by the average packing fraction.
2. Sample a flight distance of neutron.
3. Determine a material at the collision point by a flight distance and the radial distribution function of packing fraction. The radial distribution functions are prepared in prior of a STGM calculation.
4. Determine a reaction of neutron by the cross section of determined material. If a fission reaction occurs, this position is set as a new neutron source position.

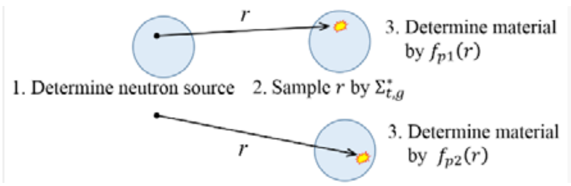

Fig. 4 Neutron random walk in the improved model.

The physical contact of fuel particles that causes fluctuation of the packing fraction is already taken into account in $f_p(r)$. Also, $f_p(r)$ is calculated in systems with random arrangement of fuel particles. Thus, improvement of calculation accuracy and efficiency can be expected compared to the current STGM model.

4. Radial Distribution Function of Packing Fraction

In the present improved STGM model, two radial distribution functions are necessary. In this section, these radial distribution functions are calculated by numerical integration by the Monte Carlo method.

Specifically, an in-house code to calculate an average packing fraction $f_p(r)$ within a distance of r is developed and used. When the Monte Carlo integration is performed from r to $r + \Delta r$, then the packing fraction in this range is expressed as follows:

$$f_p\left(r+\frac{\Delta r}{2}\right)=\frac{1}{N}\sum_{\mathrm{i}} n_i. \qquad (2)$$

n_i and N means numbers of samplings at i-th fuel particle within the integral range and all samplings within the integral range, respectively.

The radial distribution functions of packing fraction for the simple cubic lattice (SCL) and 3D random arrangement (RAND) are calculated using the above method. Table I shows calculation condition and Fig. 5 shows calculation procedure. The origin is uniformly sampled. In the case of RAND, fuel particle arrangement is also changed for different initial random seed. As an example, Fig. 6 shows the calculation example of the radial distribution function $f_{p1}(r)$ in the case of average packing fraction is 0.3.

Table I. Calculation condition to estimate radial distribution of packing fraction

N	1000
Δr [cm]	0.01
Number of iteration	1000
Fuel particle radius[cm]	1.0

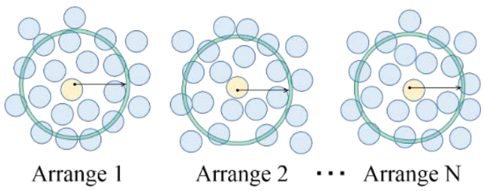

Fig. 5 Calculation procedure of $f_p(r)$.

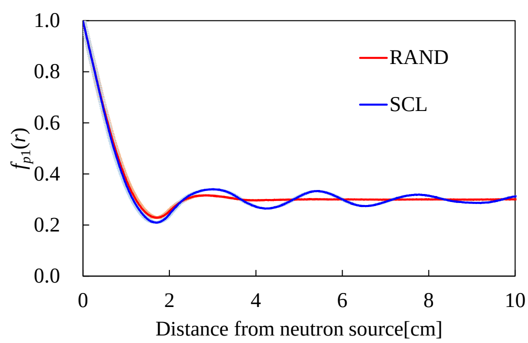

Fig. 6 Distribution function of packing fraction $f_{p1}(r)$.

In the case of SCL, Fig. 6 indicates a periodic structure which is caused by regular and periodic arrangement of fuel particle. These functions converge to the average packing fraction when the sampled flight length is longer than approximately 3cm.

5. Calculation of k-infinity using the conventional and proposed STGM models

In this section, we calculate k-infinity of a system in which fuel particles are randomly distributed in water. The conventional and the present STGM models are used. Calculation conditions are as follows: a number of neutron per batch is 10000, the active number of batches is 1000, number of energy group is 1, and the average packing fraction is 0.1, 0.2, or 0.3, the periodic boundary condition is applied for all boundaries. Verification calculation is carried out in the SCL and RAND. The radial distribution function of packing fraction is used given by the Monte Carlo integration. Table II shows macroscopic cross sections used in this calculation.

Table II. Macroscopic cross section [cm^{-1}]

	Fuel	Moderator
Σ_a	0.1	0.1
$\nu\Sigma_f$	0.1	0.0
Σ_t	0.1	0.1
Σ_s	0.0	0.0

Figures 7(a) and 7(b) show the calculation result (relative difference from the reference value) of k-infinity for SCL and the RAND. The reference value is calculated at the system where fuel particles are explicitly arranged at 3-dimensional space. In the case of RAND, 1,000 configuration with difference arrangements of fuel particles are prepared, and the mean value of k-infinity calculated from 1,000 configurations is used as the reference value. Number of configurations (1,000) is chosen to sufficiently reduce statistical error for the average value of k-infinity.

The relative difference of k-infinity is calculated as follows:

$$\Delta k_\infty=\frac{k_{calc}-k_{ref}}{k_{ref}}\times 100\ [\%] \qquad (3)$$

k_{calc} means a value of k-infinity calculated by STGM (the previous or the improved model), k_{ref} means the reference value of k-infinity.

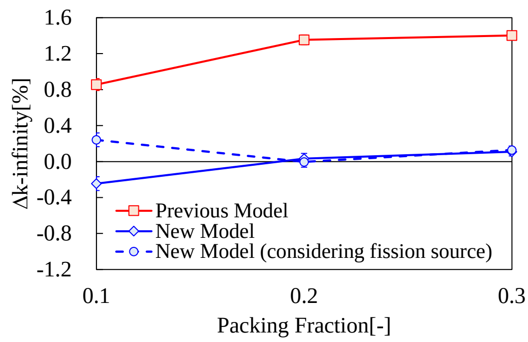

Fig. 7(a). Relative difference of k-infinity (SCL)

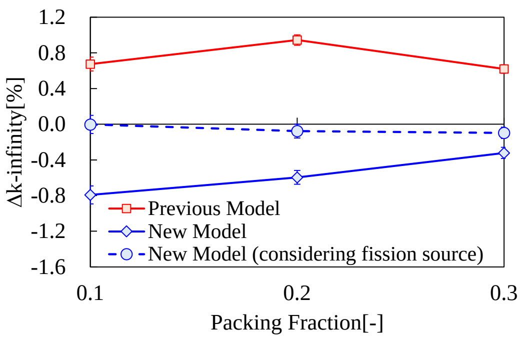

Fig. 7(b). Relative difference of k-infinity (RAND)

As shown in Fig. 7(a), calculation accuracy of proposed STGM model for SCL is better than that of previous STGM model. However, as shown in Fig. 7(b), calculation accuracy of the proposed STGM model is not significantly improved in RAND.

In the case of RAND, a packing fraction might show spatial fluctuation. Therefore, in the actual Monte Carlo calculation, the fission source distribution may show spatial dependence. For example, location where fuel particles are clouded, higher fission density would be observed. However, in the estimation of packing fraction distribution, this effect is not taken into account.

In order to consider the fission source distribution effect, we calculate the radial distribution function directly from a process of neutron random walk with explicit treatment of random distribution of fuel particles. The distribution function of $f_{p1}(r)$ considering the above effect is calculated with the following calculation conditions: the average packing fraction is 0.3, number of neutrons per batch is 10000, the active number of batches is 1000, and macroscopic cross section is Table II. Estimation result is shown in Fig. 8.

By using $f_{p1}(r)$ considering fission source distribution effect, calculation result of proposed STGM model becomes as a blue broken line. Consequently, it is clarified that calculation accuracy improves by considering fission source distribution. This result suggests that the calculation accuracy and efficiency of proposed STGM will be improved, if the fission source distribution effect can quantitatively estimate before Monte Carlo calculation.

As the result, it is clarified that the improve model can accurately estimate k-infinity of the fuel particle distribution system than the previous STGM model.

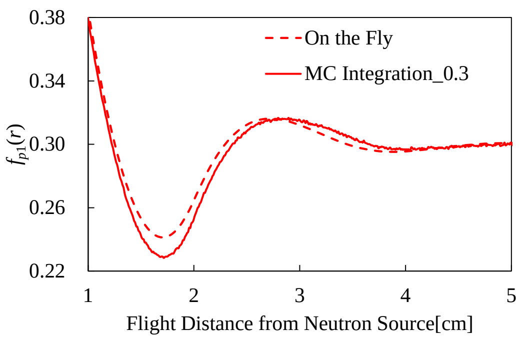

Fig. 8. $f_{p1}(r)$ in consideration of a spatial distribution of fission source.

6. Conclusions

In this study, we developed an improved statistical geometry model with the delta-tracking method. In the previous STGM model, flight analysis of neutron is carried out using the nearest neighbor distribution. In the present study, we simplify the calculation algorithm using the radial distribution function of a packing fraction.

K-infinity obtained by the present improve and previous STGM models are compared with reference value. The calculation results indicate that prediction accuracy of the improved model is higher than that of the previous model.

As a future work, further verifications of the proposed STGM model and consideration of computing time will be carried out.

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