A Proposal of New Spherical Particle Modeling Method Based on Stochastic Sampling of Particle Locations in Monte Carlo Simulation

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1. Introduction

The design concepts of the randomly distributed spherical particles have been utilized for the VHTR reactors, shielding materials, and blanket design in the fusion reactors. In Monte Carlo (MC) simulation, the explicit modeling of all random spherical particles cannot be fully performed because of the numerous numbers of the particles as well as the random positions of the particles. Implicit method is a modeling method of the spherical particles that is based on the sampling of the particle geometry during the MC simulation [1, 2]. Due to the high computational efficiency and user convenience, the implicit method had received attention; however, it is noted that the implicit method in the previous studies has low accuracy at high packing fraction [2]. In this study, a new implicit method, which can be used at any packing fraction with high accuracy, is proposed.

2. Methods and Results

2.1 Proposal on Particle Sampling Method

The basic concept of the proposed particle modeling method in a random particle distributed medium is based on the geometrical cross section of the spherical particle [3]. The particle has spherical shapes; hence, the microscopic cross section and the number density of the medium are given as the following:

$$\sigma_p = \pi r_p^{\ 2} \tag{1}$$

$$N_p = n / V_m \tag{2}$$

where, r_p is the radius of the particle, n is number of particle in unit volume V_m. The distance l_p of the new particle location from the current neutron position can be sampled by Eq. (4).

$$\Sigma_p = N_p \sigma_p \tag{3}$$

$$l_p = -\frac{1}{\Sigma_p}\ln(\xi_0) \tag{4}$$

where, ξ_0 is a random number. By using the distance, new position (x_1, y_1, z_1) of the sampled spherical particle is determined by Eq. (5).

$$\begin{aligned} x_1 &= x_0 + l_p u_0 + r_p\sqrt{\xi_1}\,\frac{\xi_2 u_0 v_0 - \xi_3 v_0}{\sqrt{(\xi_2^2+\xi_3^2)(1-w_0^2)}} \\ y_1 &= y_0 + l_p v_0 + r_p\sqrt{\xi_1}\,\frac{\xi_2 v_0 w_0 - \xi_3 u_0}{\sqrt{(\xi_2^2+\xi_3^2)(1-w_0^2)}} \\ z_1 &= z_0 + l_p w_0 + r_p\sqrt{\xi_1}\,\frac{\xi_2\sqrt{1-w_0^2}}{\sqrt{\xi_2^2+\xi_3^2}} \end{aligned} \tag{5}$$

where, (x_0, y_0, z_0) is the current neutron position, (u_0, v_0, w_0) is the unit vector of neutron transport direction, and ξ_1, ξ_2, ξ_3 are the random numbers. After the position of the spherical particle is sampled, previous particle is removed. Also, the particle sampling is rejected when the particle is sampled at the boundary of the particle distributed medium.

In using the proposed modeling method, an overlapping problem of the sampled particle with previous particle position is generated as shown in Figure 1 (yellow sphere). To correct the position of the sampled sphere, it is assumed that the sampled particle, which is overlapped with initial sphere, is moved to the contact point of the initial spherical particle on the neutron direction as given in Eq. (6).

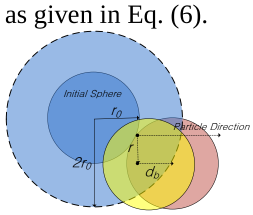

Fig. 1. Overlap of the Sampled Spherical Particle (Yellow Sphere) and Corrected Position (Red Sphere)

$$\begin{aligned} x_1 &= x_0 + d_b u_0 + r_p\sqrt{\xi_1}\,\frac{\xi_2 u_0 v_0 - \xi_3 v_0}{\sqrt{(\xi_2^2+\xi_3^2)(1-w_0^2)}} \\ y_1 &= y_0 + d_b v_0 + r_p\sqrt{\xi_1}\,\frac{\xi_2 v_0 w_0 - \xi_3 u_0}{\sqrt{(\xi_2^2+\xi_3^2)(1-w_0^2)}} \\ z_1 &= z_0 + d_b w_0 + r_p\sqrt{\xi_1}\,\frac{\xi_2\sqrt{1-w_0^2}}{\sqrt{\xi_2^2+\xi_3^2}} \end{aligned} \tag{6}$$

where, d_b is the distance from the sampled position to the contact point with the initial spherical particle.

2.2 Corrections of Number Density

Due to the rejection method, the number density, N_p, is changed during the sampling simulation. To correct the number density, the following definition is used:

i) The number density in Region A is constant.
ii) The number density is gradually decreased at the boundary of the particle distributed medium due to the particle sampling rejection at the purple color region.

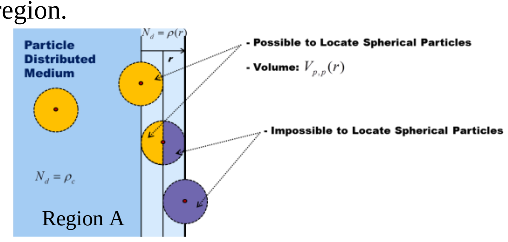

Fig. 2. Change of Number Density at Boundary of Medium

From the definitions, the number density at the boundary can be calculated by the Eq. (7).

$$\rho(r) = \frac{V_{p,p}(r)}{V_{T,p}}\rho_c \tag{7}$$

where, ρ_c is the number density at Region A, $V_{T,p}$ is the volume of the spherical particle, $V_{p,p}(r)$ is the local region volume of which the sampled particle can be located. The $V_{p,p}(r)$ is differently calculated with the boundary types which are plate, cylinder, and sphere. The calculation results are given in Eqs. (8), (9), and (10) for plate, cylinder, and sphere, respectively.

$$V_{p,p}(r) = \frac{4}{3}\pi r_p^{\ 3} - \pi r_p r^2 + \frac{1}{3}\pi r^3 \tag{8}$$

$$V_{p,p}(r) = V_{p,cy}(r) \approx \Delta z \sum_{i=1}^{n} \begin{bmatrix} \frac{\pi}{2} R'^2 - p(r,z)\sqrt{R'^2 - p(r,z)^2} - R'^2 \arcsin[\frac{p(r,z)}{R'}] \\ \frac{\pi}{2} r_p(z)^2 - \{r - p(r,z)\}\sqrt{r_p(z)^2 - \{r - p(r)\}^2} \\ -r_p(z)^2 \arcsin[\frac{\{r - p(r)\}}{r_p(z)}] \end{bmatrix} \tag{9}$$

$$V_{p,p}(r) = \pi\left(\frac{2}{3}R'^3 - R'^2\ p(r) - \frac{1}{3}p(r)^3 + \frac{2}{3}r_p^{\ 3} - r_p^{\ 2}(r - p(r)) - \frac{1}{3}(r - p(r))^3\right) \tag{10}$$

where, *R'* is (r_p-R_c), R_c is the cylinder or sphere radius of the particle distributed medium, $p(r)$ or $p(r,z)$ is the intersection position between the spherical particle and particle distribution surfaces, Δz is the unit distance for using the numerical method.

Also, the movement of the overlapped particle causes the change of the number density. For the collection, an empirical method in the previous study [3] is used. At first, the particle sampling calculations with the proposed method were performed as increase of the number density. And then, the number densities, which are measured in each calculated, are recorded. The calculation results are shown in Figure 3.

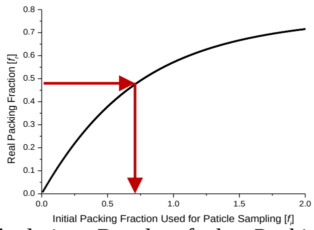

Fig. 3. Calculation Result of the Packing Fraction with Proposed Method

As shown in Figure 3, the number density is changed due to the particle movement; hence, the collection of the packing fraction must be performed. The number density collection for the use in the particle sampling simulation is calculated by Eqs. (11) and (12).

$$f_i = f_{i,j+1} - \frac{f_{i,j+1} - f_{i,j}}{f_{r,j+1} - f_{r,j}}\left(f_{r,j+1} - f_r\right) \tag{11}$$

$$N_{pc} = \frac{f_i}{f_r} N_p \tag{12}$$

where, f_i is the packing fraction used the particle sampling, f_r is the calculated packing fraction with f_i, and j is bin number.

2.3 Verification of Proposed Sampling Method

For the verification, the particle sampling simulations with the proposed method were pursued in infinite (Table I) and finite mediums (Table II). The spherical particle, which has 3 cm radius, is continually sampled in the mediums until 10^7 times in the infinite and finite mediums. The simulation was performed C++ program, and all results have < 0.1 % stochastic errors. The results show that the proposed method can accurately simulate the spherical particles within 0.1 % relative difference.

Table I. Calculation Result of the Packing Fraction in the Infinite Medium

Initial PF	Calculated PF	Relative Difference	Initial PF	Calculated PF	Relative Difference
0.05	0.049985	-0.03%	0.40	0.400055	+0.01%
0.10	0.100014	+0.01%	0.45	0.450028	+0.01%
0.15	0.150010	+0.01%	0.50	0.500047	+0.01%
0.20	0.199981	-0.01%	0.55	0.550060	+0.01%
0.25	0.250015	+0.01%	0.60	0.599962	-0.01%
0.30	0.300011	+0.00%	0.65	0.649999	-0.00%
0.35	0.350001	+0.00%	0.70	0.699960	-0.01%

Table II. Calculation Result of the Packing Fraction in Finite Mediums (Cubic, Cylinder, and Sphere)

PF	Cubic			Cylinder			Sphere		
	100 cm	200 cm	500 cm	100 cm	200 cm	500 cm	100 cm	200 cm	500 cm
0.1000	0.1001	0.0994	0.0996	0.0999	0.1000	0.1000	0.0999	0.1000	0.1000
0.2000	0.1999	0.1987	0.1993	0.1998	0.1999	0.2000	0.1998	0.1999	0.2000
0.3000	0.3000	0.2982	0.2989	0.2996	0.2999	0.2999	0.2996	0.2998	0.2999
0.4000	0.4006	0.3978	0.3987	0.3993	0.3997	0.3999	0.3994	0.3998	0.4000
0.5000	0.5025	0.4977	0.4984	0.4992	0.4996	0.4999	0.4994	0.4997	0.4999
0.6000	-	0.5985	0.5983	0.5990	0.5995	0.5999	0.5994	0.5996	0.5999

3. Conclusions

In this study, the implicit modeling method in the spherical particle distributed medium for using the MC simulation is proposed. A new concept in the spherical particle sampling was developed to solve the problems in the previous implicit methods. The sampling method was verified by simulating the sampling method in the infinite and finite medium. The results show that the particle implicit modeling with the proposed method was accurately performed in all packing fraction boundaries. It is expected that the proposed method can be efficiently utilized for the spherical particle distributed mediums, which are the fusion reactor blanket, VHTR reactors, and shielding analysis.

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REFERENCES

[1] Murata I., et. al., “New Sampling Method on Continuous Energy Monte Carlo Calculation for Pebble Bed Reactor,” Joumal of Nuclear Science and Technology, 34(8), 734-744, 1997.

[2] Jaakko Leppänen, “PSG2 / Serpent – a Continuous-energy Monte Carlo Reactor Physics Burnup Calculation Code,” VTT Technical Research Centre of Finland, 2009.

[3] S. H. KIM et al., “A Development of Monte Carlo Evaluation Method with Particle Sampling Techniques for Pebble Bed Reactor,” Nuclear Technology, Vol. 177, p. 147-156, 2012.