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An Analysis of Spherical Particles Distribution Randomly Packed in a Medium for the Monte Carlo Implicit Modeling

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1. Introduction

Spherical particles, which are randomly distributed in medium, are utilized for the radiation shields, fusion reactor blanket, fuels of VHTR reactors. Due to the difficulty on the simulation of the stochastic distribution, Monte Carlo (MC) method has been mainly considered as the tool for the analysis of the particle transport. For the MC modeling of the spherical particles, three methods are known; i) repeated structure[1], ii) explicit modeling[2], and iii) implicit modeling[3]. Implicit method (called as the track length sampling method) is a modeling method that is the sampling based modeling technique of each spherical geometry (or track length of the sphere) during the MC simulation. Implicit modeling method has advantages in high computational efficiency and user convenience [3]. However, it is noted that the implicit method has lower modeling accuracy in various finite mediums [4]. In this study, as a preliminary study to develop an implicit method having high accuracy, the distribution characteristics of spherical particles were evaluated by using explicit modeling techniques in various volume packing fractions.

2. Methods and Results

First, to analyze the distribution characteristics, an explicit modeling method by the modification of random sequential addition (RSA) [5] was developed as shown in Section 2.1. Using the explicit modeling method, the characteristics of the spherical particle distribution were evaluated in Section 2.2.

2.1 Explicit Monte Carlo Modeling of Randomly Packed Spheres

To evaluate the characteristics of the spherical particle distribution, a medium was set to 102 cm x 22 cm x 22 cm hexahedron. The radius of the spherical particles, which are filled in the medium, is assumed to be 1 cm. For the particle sampling, the particle sampling with the modified RSA method, which is proposed in this study, is performed as the following procedure:

i) A position of sphere is sampled with RSA method.
ii) If a particle is overlapped with the previous particle, the positions of the overlapped particles are moved by Eq. (1).
iii) If a particle is located out of medium boundary, the position is rejected, and a new position is sampled.
iv) The process was repeated until all of spheres were not overlapped and located in the accepted boundary.

$$x_1' = x_1 - lu \quad (1\text{-a})$$

$$y_1' = y_1 - lv \quad (1\text{-a})$$

$$z_1' = z_1 - \hat{l}w \quad (1\text{-a})$$

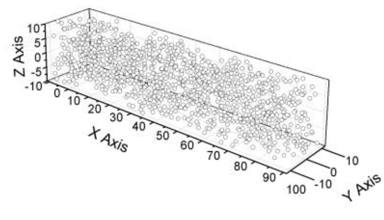
$$x_2' = x_2 + \hat{l}u \quad (1\text{-a})$$

$$y_2' = y_2 + \hat{l}v \quad (1\text{-a})$$

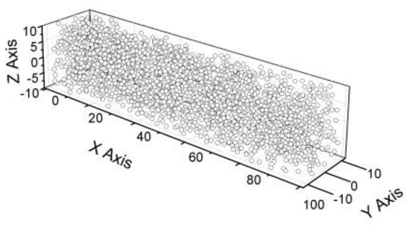
$$z_2' = z_2 + \hat{l}w \quad (1\text{-a})$$

where (x_1, y_1, z_1) and (x_2, y_2, z_2) are positions of the overlapped spheres, (u, v, w) is the unit vector from center of particle #1 to center of particle #2, and l is a user defined length to avoid the overlap.

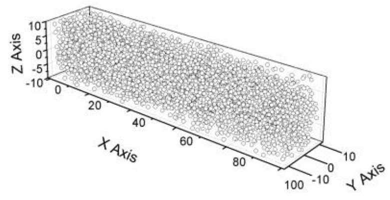
For the analysis of the particle distribution, four cases of the packing fraction were modeled. Figure 1 shows the modeling results of randomly packed spheres using MATLAB program.



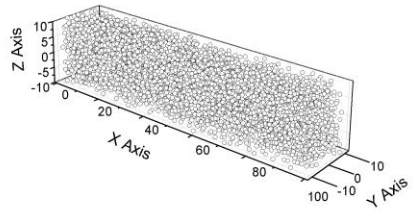
(a) 10 % Packing Fraction



(b) 20 % Packing Fraction



(c) 30 % Packing Fraction



(d) 40 % Packing Fraction

Fig.1. Modeling Result of Randomly Packed Spheres Using Proposed Method

2.2 Analysis of the Distribution Characteristics

In the previous studies [3, 6], the probability distribution of the sampled particle length for the implicit modeling was assumed to have an exponential function. For analyzing the distribution characteristics to verify the assumption, explicit modeling was performed using the modified RSA method described in Section 2.1. It is noted that the packing fraction of spheres are gradually decreased as approaching the wall boundary [7]. Therefore, the packing fraction near the wall boundary is a variable as the particle location. To avoid the wall boundary effect, the packing fraction in the center region is used for the distribution analysis. For the hexahedron geometry, the center region is given in Figure 2. It is noted that the packing fraction in the center region has higher value than the average packing fraction. To calculate the packing fraction of center region, a track length estimation method was used. The results of the packing fraction in center region are calculated as shown in Table I.

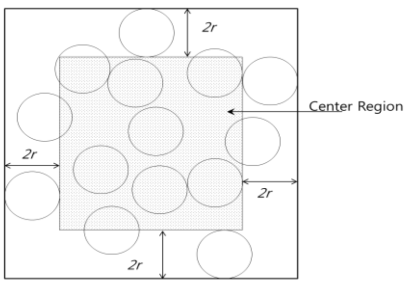


Fig.2. Center Region in the Hexahedron Medium

Table I: Packing Fraction in Center Region

Average PF	PF in Center Region	σ
0.1	0.12515	0.00035
0.2	0.25181	0.00062
0.3	0.37389	0.00047
0.4	0.49834	0.0006

To verify the implicit modeling method, the distributions of l_p and r_p, which are used in the previous sampling method [7], are calculated in the medium. The brief description about l_p and r_p is shown in Figure 4.

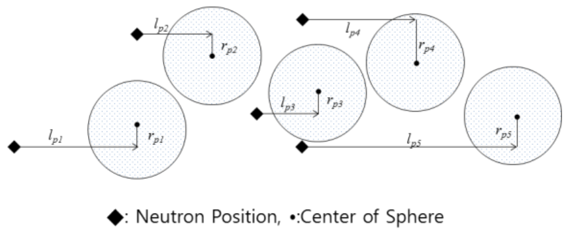
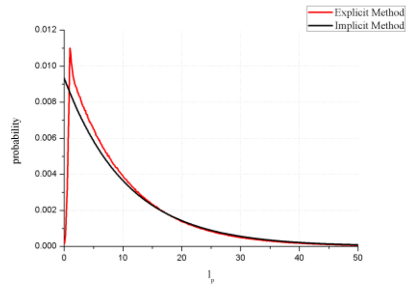
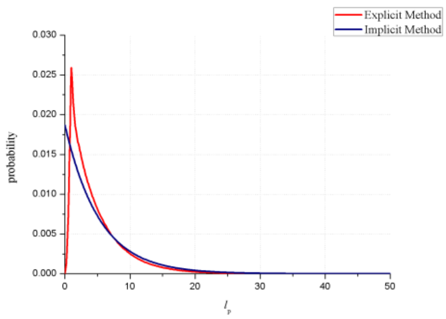


Fig.3. Description of l_p and r_p

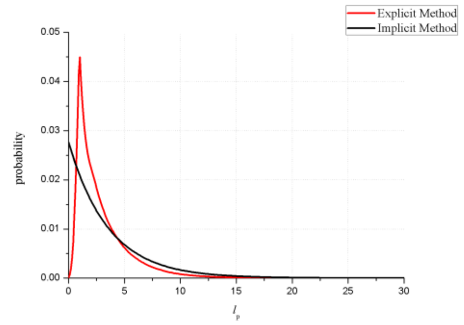
Using the proposed method, 100 cases for each packing fraction were generated for the medium described in Section 2.1. Then, the 10^5 starting positions are randomly sampled and the l_p and r_p are estimated in each case. Also, using the implicit method proposed by previous study [6], the l_p was estimated for each packing fraction. Figure 4 shows the l_p results for each packing fraction with the explicit modeling and implicit modeling methods. Analysis shows that the implicit method can give a large error as increasing the packing fraction.



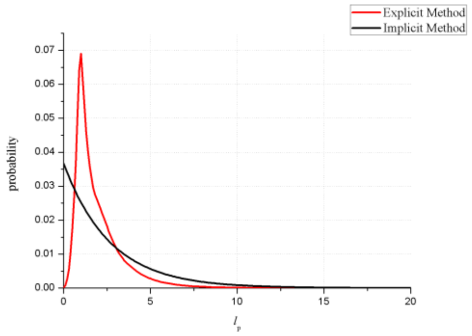
(a) 10 % Packing Fraction



(b) 20 % Packing Fraction



(c) 30 % Packing Fraction



(d) 40 % Packing Fraction

Fig.4. Comparing explicit l_p distribution with implicit l_p distribution.

Also, the results of average r_p as the l_p distance were estimated shown in Figure 5. In the implicit method, it is assumed that r_p is fixed to a value. However, the result shows that the r_p can be changed within radius of the particle.

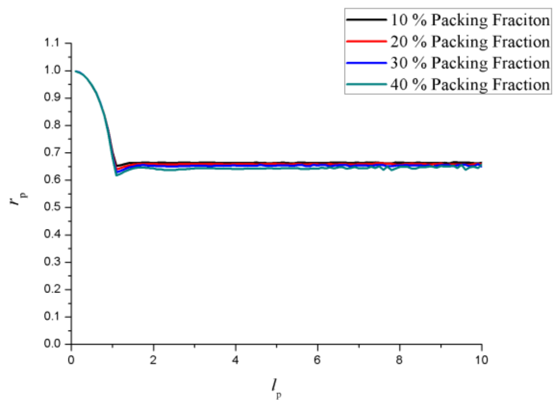


Fig.5. Distribution of Average r_p along l_P

3. Conclusions

This study was performed to evaluate implicitly simulated distribution of randomly packed spheres in a medium. At first, an explicit modeling method to simulate random packed spheres in a hexahedron medium was proposed. The distributed characteristics of l_p and r_p, which are used in the particle position sampling, was estimated. It is analyzed that the use of the direct exponential distribution, which is generally used in the implicit modeling, can cause the distribution bias of the spheres. It is expected that the findings in this study can be utilized for improving the accuracy in using the implicit method.

4. Acknowledgement

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