Numerical Simulation of Particle Infiltration using Pseudo Three-Dimensional Distinct Element Method

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Abstract

A low-decontaminated Mixed Oxide (MOX) fuel which includes high radioactive rare earth elements and Minor Actinides (MA) will be a main candidate for Fast Breeder Reactor (FBR) cycle. From the viewpoint of a prevention of radiation exposure and lower manufacturing cost in the fuel fabrication system, a sphere-pac fuel manufacturing and vibro-filling process is to be promising. In the process, spherical shaped fuels of different diameters are packed into a fuel pin and are infiltrated and thickened by vibration. For achieving a high and uniform packing density, it is needed to comprehend the infiltration phenomena and to evaluate an influence of the vibration, such as a frequency and amplitude, on the packing density.

A Distinct Element Method (DEM), which is a technique to analyze a dynamic behavior of discontinuous element's aggregation, has been applied. A typical three-dimensional DEM, in which an infiltration phenomenon can be simulated successfully, requires significant computational resources. Hence, a new concept of pseudo three-dimensional DEM was developed. A virtual diameter, which can be calculated based on an orthographic projection of three-dimension onto two-dimension, is introduced in a two-dimensional DEM in order to judge the contact criterion and calculate the interactive forces between the particles.

In the present study, sensitivity analyses of frequency and amplitude in the vibration has been carried out using the developed method. The comparison between the pseudo three-dimensional DEM and a three-dimensional DEM has also been carried out.

Keywords

Distinct Element Method, Sphere-Pac, Pseudo Three-Dimension, Fuel fabrication

1. **INTRODUCTION**

In a development of Fast Breeder Reactor (FBR) cycle in Japan, a low decontaminated Mixed Oxide (MOX) fuel in which Minor Actinides (MA) is included will be fabricated. During the fabrication, it is required to eliminate radiation exposure of workers as well as to achieve low manufacturing cost. One of possible candidates is a sphere-pac fuel manufacturing and vibro-filling process. In the process of sphere-pac fuel production, fuel is formed to be spheral and it is filled in a cladding tube under a vibration motion. In the sphere-pac fuel manufacturing, complicated processes are not required, such as atomization of fuel and a sintering of fine powder to form a fuel pellet, resulting in low manufacturing cost. At the same time, the prevention of the radiation exposure can be achieved by its easy remote handling.

In the process, particles of different diameters are blended by adding external vibration as shown in Fig. 1. In order to obtain a high and uniform packing density in the fabrication, experimental works has been carried out [1], [2]. However, one needs to comprehend the behavior of the particles in a vibrating tube to estimate an influence of the vibration condition such as amplitude and frequency. Consequently, a development of numerical simulation method for the vibro-filling process is of importance.
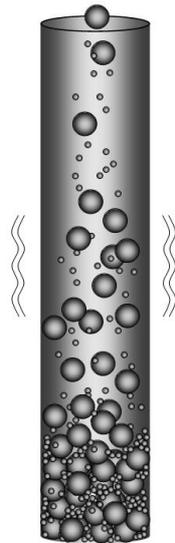

Fig. 1 Schematic of Vibro-Filling System

The Distinct Element Method (DEM) is a technique to simulate a dynamic behavior of discontinuous element's aggregation [3]. A three-dimensional (3D) DEM has a great advantage to investigate infiltration phenomena, while it requires significant computational resources. Accordingly, the authors developed the numerical simulation method using a pseudo 3D DEM [4] in which an infiltration of small particles through large particles can be analyzed even in a two-dimensional calculation.

In the present study, a comparison between the pseudo 3D and 3D DEMs has been carried out to estimate an applicability of the developed method. Parameter study of the vibration condition such as amplitude and frequency has been also carried out to investigate an efficient packing manner.

2. PSEUDO THREE-DIMENSIONAL DEM

2.1 Summary of DEM

In the DEM, the Newton's second law of each particle is solved successively. As an example of two-dimensional DEM, the following governing equations are taken into consideration.

$$m\frac{d^2x}{dt^2} = \sum_{j=1}^{n} F_{xj} \tag{1}$$

$$m\frac{d^2y}{dt^2} = \sum_{j=1}^{n} F_{yj} - mg \tag{2}$$

$$I\frac{d^2\psi}{dt^2} = \sum_{j=1}^{n} F_{\psi j} \cdot r_j \tag{3}$$

Where, m, r and I mean the mass, the radius of particle and the inertia moment respectively. x, y and ψ are the x- and y-coordinates and the rotational displacement respectively. F is the contact force and n is the number of contact particles. With regard to the contact force, the Voigt model, in which a virtual spring and a virtual dashpot are parallely-connected, is applied as shown in Fig. 2. It is mentioned that a frictional slider that represents a kinetic friction is introduced in the tangential direction.
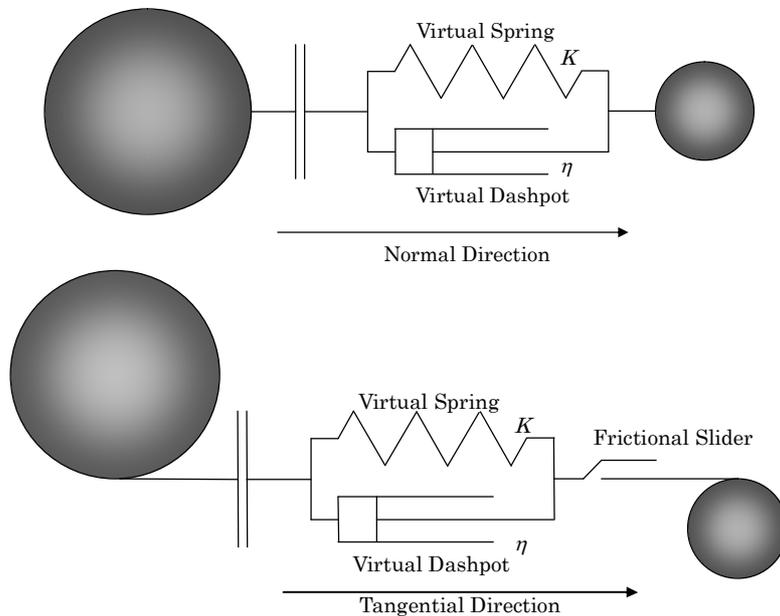

Fig.2 Voigt Model

The virtual spring means the repulsion and friction force being proportional to relative displacement of two particles. Kinetic energy dissipation due to relative velocity between the particles is expressed by the virtual dashpot. As a result, one obtains the following contact forces along the normal and the tangential directions as;

$$F_n = \eta_n \frac{du_n}{dt} + K_n u_n \tag{4}$$

$$F_t = \eta_t (\frac{du_t}{dt} + r\frac{d\psi}{dt}) + K_t(u_t + r\psi) \tag{5}$$

here, h and K are the damping coefficient and the stiffness coefficient. u is the relative velocity. Subscripts n and t show the normal and the tangential directions. The contact forces of Eqs. (4) and (5) are transformed in horizontal (x), vertical (y) and rotational (ψ) components in the global coordinates.

In case of 3D DEM, a contact decision becomes complicated rather than that in two-dimension and a number of contacts arises at each computational time step. Furthermore, an increase of the degree of freedom requires the increase of the governing equations. Consequently, a significant computational cost is needed in 3D DEM. At the same time, an infiltration phenomenon cannot be represented in two-dimensional DEM [5]. Hence, a pseudo 3D treatment has been introduced so as to simulate the infiltration phenomenon with a reasonable computational cost.

2.2 Pseudo Three Dimensional Model

In the pseudo 3D DEM [4], a concept of virtual radius which is calculated based on an orthographic projection of three-dimension onto two-dimension is introduced. A specified geometrical configuration is taken into account for simplicity.

With regard to the virtual radius between the same size particles, a closest packing lattice is assumed. Figure 3 shows the orthographic projection. As shown in Fig. 3, particles penetrate into adjoining particles at the two-dimensional projection. The virtual radius (r') is obtained from the geometrical configuration ($r' = (\sqrt{11/3} - 1)r$).
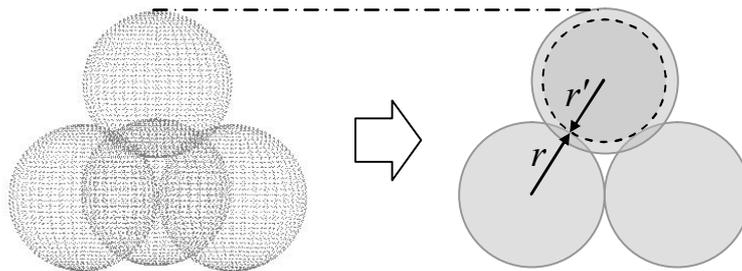

Fig. 3 Orthographic Projection of Same Particles Size (side view)

In case of the infiltration of fine particle through a gap, the virtual radius ($r_c' = (2 - 2\sqrt{3}/3)r_c$) is applied only to a coarse particle and is calculated based on an equilateral-triangular displacement that consists of adjoining coarse particles as in Fig. 4. Here, r_c is the radius of the coarse particle.

Consequently, it can also be said that the coarse particles and fine particles in the present pseudo 3D DEM model are allocated along to the barycentric lines in actual three-dimensional coordinates as in Fig. 5.

Using the virtual radius, the contact criterion between particles is checked and the contact forces in Eqs. (4) and (5) are calculated. After the transformation of the contact forces into the global coordinates, the governing equations are solved based on the actual radius. The second order Adams-Bashforth method is applied as a numerical solution.
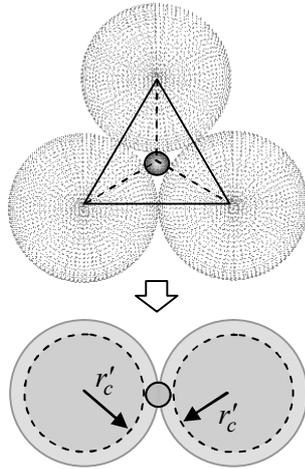

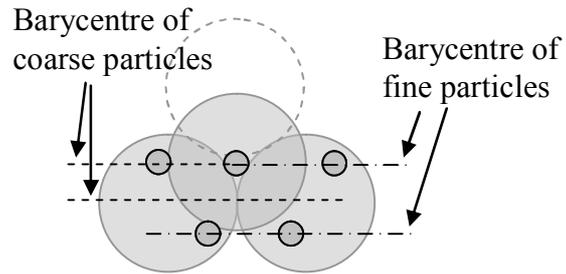**Fig. 4 Orthographic Projection of Different Particles Size (side view)**

Fig. 5 Particle allocation in pseudo three-dimensional model (top view)

3. NUMERICAL SIMULATION OF PARTICLE INFILTRATION

Two kinds of numerical simulation have been carried out to investigate an applicability of the present model and a sensitivity of vibrating condition on the packing density. In both analyses, the dimension of the particle diameter and the container is assumed to be similar to those of the practical fuel fabrication [2] but less number of the particles is considered in the analyses for simplicity. Table 1 shows the geometrical condition and the material properties.

Table 1 Geometrical Condition and Material Properties

Particles		
Diameter	[m]	Coarse 1.4×10^{-3}, Fine 2.0×10^{-4}
Density	[kg/m^3]	1.1×10^{4}
Young's modules	[Pa]	1.0×10^{10}
Poisson's ratio	[-]	0.28
Coefficient of friction	[-]	0.25
Coefficient of rebound	[-]	0.80
Container		
Width (W)	[m]	1.0×10^{-2}
Young's modules	[Pa]	3.9×10^{10}
Poisson's ratio	[-]	0.25
Coefficient of friction	[-]	0.17

3.1 Comparison between Pseudo Three-Dimensional and Three-Dimensional Analyses

In the comparison between the present pseudo 3D and 3D DEMs, the distribution of packing density along the vertical axis and the conformation of the particles at the top of the heap have been investigated as well as the computational cost.

Figure 6 indicates the geometry of the container adopted to 3D DEM. Since the disagreement due to the methodology is investigated in the present study, the rectangular container is set in the 3D DEM analysis. In addition, a half width comparing with the pseudo 3D analysis is assumed because of the computational cost. It is noted that a symmetric boundary condition is considered at the right side wall of the three-dimensional analysis in terms of barycentric particle motion. Hence the width of container varies with the particle size as;

$$W_c = \frac{W}{2} + r_c, \; W_f = \frac{W}{2} + r_f \tag{6}$$

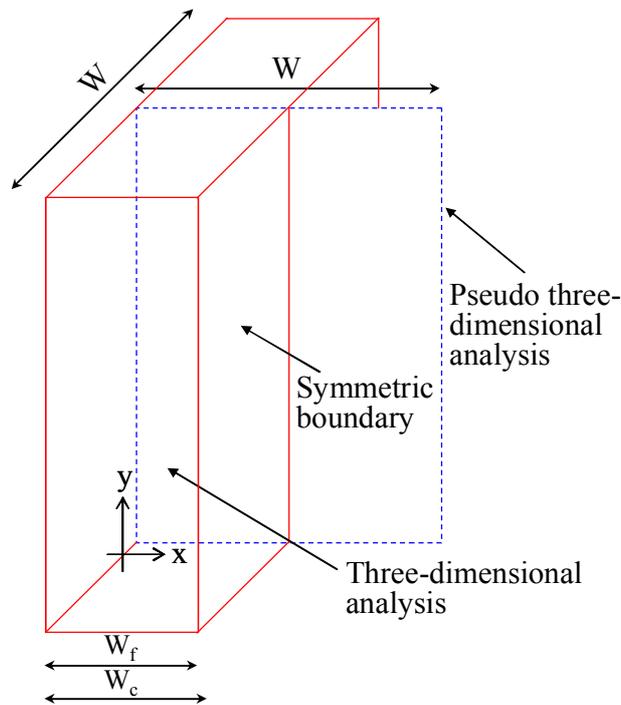Here, subscript f means the fine particle.

Fig. 6 Analytical Geometry

In case of the pseudo 3D DEM, 26 coarse particles and 1500 fine particles are embedded, whereas 36 coarse particles and 3000 fine particles are assigned in the 3D DEM. In both analyses, the coarse particles are set as a closest packed lattice firstly. Then the fine particles are fed from the top side of the container adding a vibration of the container. The computational time step and analytical duration are set to 1.0×10^{-7} and 1.0sec respectively. With regard to the vibrating condition, a sine curve is assigned. The amplitude (a) is selected as a parameter and is set to 5.0×10^{-5} and 7.5×10^{-5} m. On the other hand, a constant frequency ($f = 200$Hz) is adopted.

The comparisons of the snap shot of the particles motion are summarized in Fig. 7. When the amplitude of the vibration is smaller ($=5.0\times10^{-5}$), the coarse particles are not dispersed less than that in case of the high amplitude ($=7.5\times10^{-5}$) in both DEM computations. As seen in Fig. 7, it can be said that the qualitative nature of the particle behavior is well simulated in the present pseudo 3D DEM although the fine particles seems to be infiltrated more in the pseudo 3D analysis. This is attributed the fact that the fine particles are allocated virtually at the center of the equilateral-triangular displacement of the coarse particles lattice (see Fig. 5). Besides, the virtual allocation is clearly visualized in Fig. 7. It is noted that the actual number of infiltrated fine particles in the 3D DEM is much more than the pseudo 3D analysis.
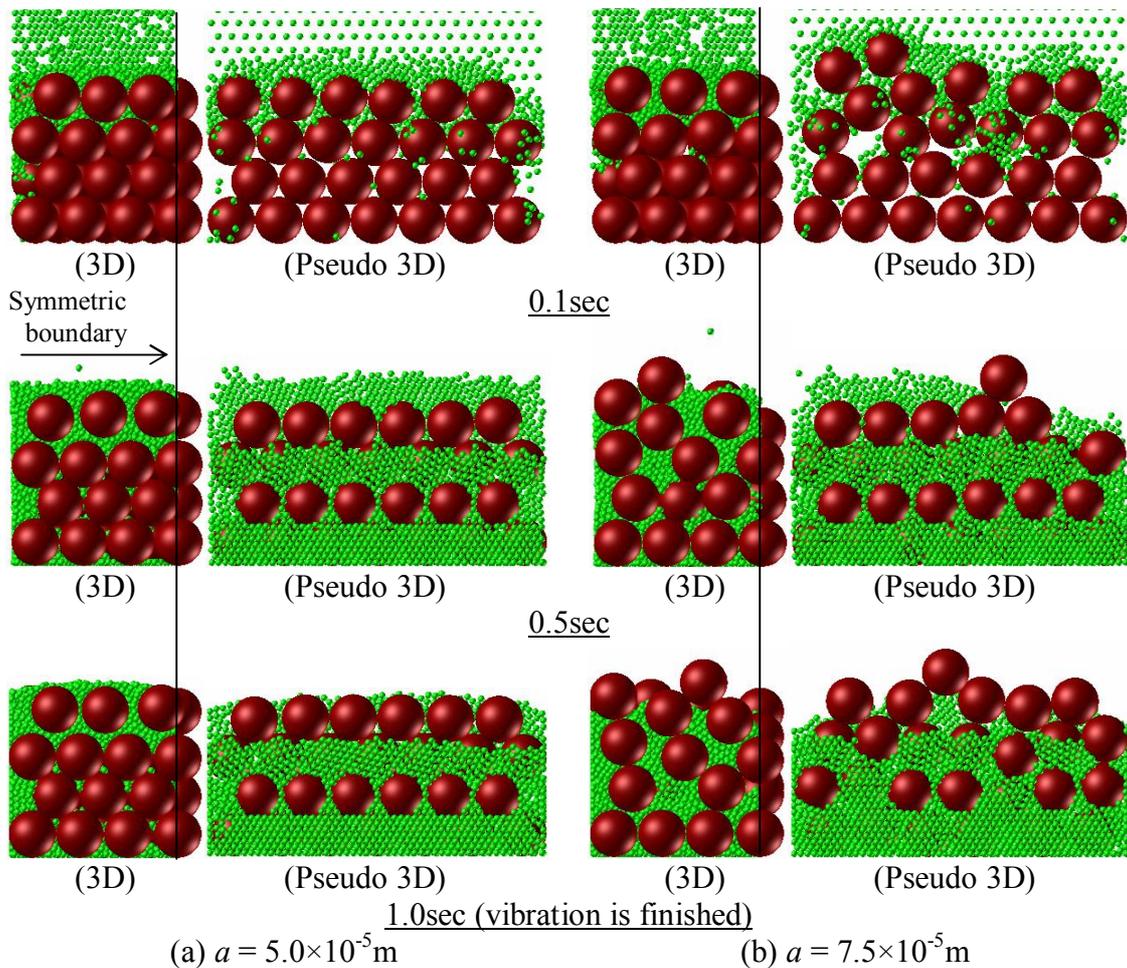

(3D)   (Pseudo 3D)   (3D)   (Pseudo 3D)

Symmetric boundary →

0.1sec

(3D)   (Pseudo 3D)   (3D)   (Pseudo 3D)

0.5sec

(3D)   (Pseudo 3D)   (3D)   (Pseudo 3D)

1.0sec (vibration is finished)

(a) $a = 5.0\times10^{-5}$m   (b) $a = 7.5\times10^{-5}$m

Fig. 7 Comparison of Particles Motion

Figure 8 shows the packing density along to the vertical axis at $a=7.5\times10^{-5}$m. The packing density is calculated based on the Monte Caro method. In case of the pseudo 3D DEM, the actual allocation shown in Fig. 5 is considered to evaluate the packing density. A dashed line in Fig. 8 corresponds to the barycentric line of the coarse particles where the closest packed lattice is achieved.

As in Fig. 8, a local maximum of the packing density appears near the barycentric lines in both analyses. It seems that the alignment of the coarse particles affects the maximum packing density in the vibro-filling fabrication. As seen in Fig. 5, only a certain

probability of the particle allocation is taken into consideration in the present model. As a result, a lower packing density is predicted as shown in Fig. 8. However, a qualitative tendency of the packing density agrees with that of the 3D DEM.

As concerns the computational cost, it is concluded that approximately one tenth of the computational cost is required in the pseudo 3D DEM comparing with the 3D DEM. Although the quantitative agreement between the pseudo 3D and the 3D DEMs is still challenging, the present model has a great advantage that the vibro-filling process of the fuel fabrication can be investigated unlike a two-dimensional DEM. Furthermore, it requires less computational cost than 3D DEM.
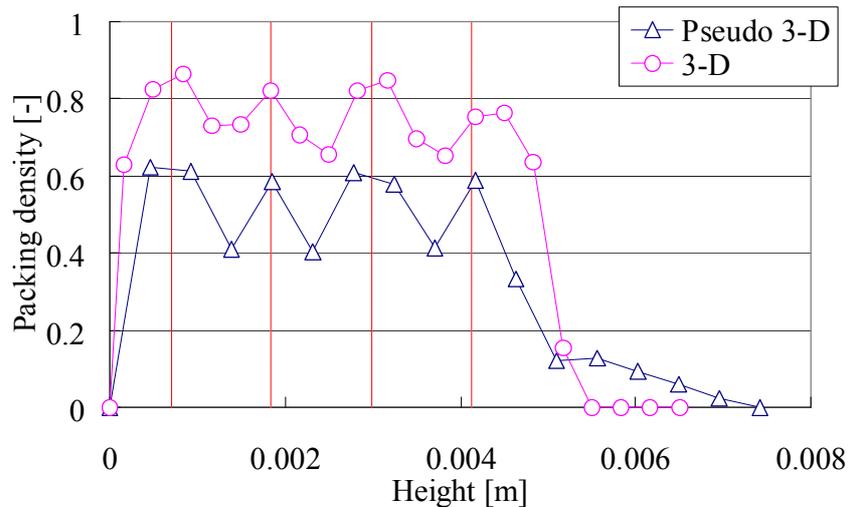

Fig. 8 Packing Density along Vertical Axis (a=7.5×10^{-5}m)

3.2 Sensitivity Analysis of Vibrating Condition

As a sensitivity study of vibrating condition on the average packing density, parametric analyses of the frequency (f) and the amplitude (a) are carried out using the pseudo 3D DEM. In the analyses, the frequency and the amplitude vary from f = 0Hz, a = 0m to f = 300Hz, a = 1.5×10^{-4}m. The other conditions are the same with Section 3.1.

Figures 9 and 10 show the influence of the amplitude (a) and the frequency (f) on the average packing density, respectively. It is noted that the packing density is averaged from y = 7.0×10^{-4}m to y = 3.0×10^{-3}m where the first and the third local maximum of the packing density appear (see Fig. 8). As seen in Figs. 9 and 10, the similar tendency of the average packing density is predicted in terms of both the amplitude and the frequency. When the amplitude or the frequency becomes lower, the lower packing density is obtained. In the similar way, the lower packing density is investigated as the value of the amplitude and the frequency becomes higher. Thus the most appropriate vibrating condition will exist in the analyses.

This can be explained from the view point of the kinetic energy transfer from the container to the particles. As a result of the container vibration, kinetic energy transfers to the particles by colliding with the wall. When the added kinetic energy is small, the alignment of, especially, coarse particles cannot be dispersed and less infiltration takes

place. On the other hand, the alignment of the coarse particles will be dispersed easily in case of high kinetic energy transfer. Therefore a number of particles will be distributed widely in total rather than clinging each other resulting in a thin packing density seen in Fig. 7(b).
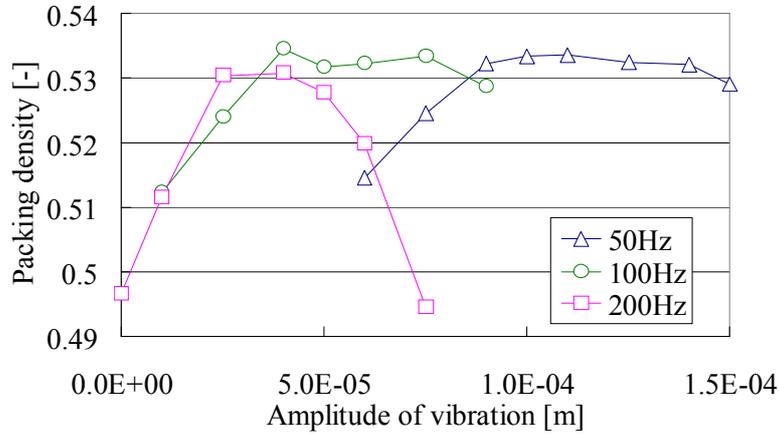

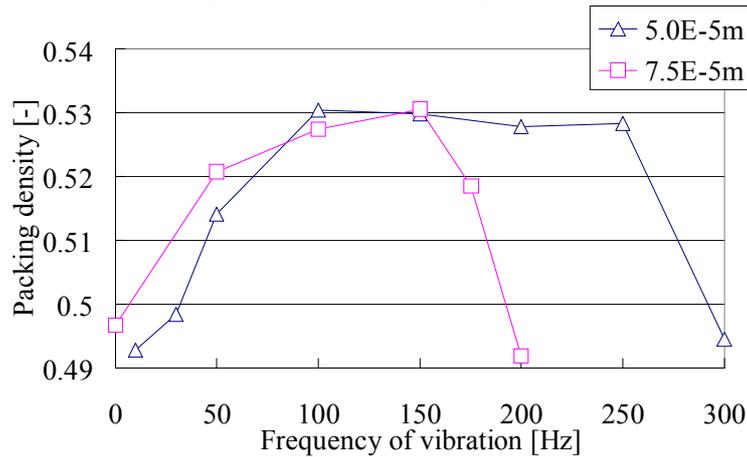**Fig. 9 Influence of Amplitude**

Fig. 10 Influence of Frequency

Let us discuss a simple assumption with regard to the kinetic energy. Kinetic energy produced by vibration can be expressed as;

$$k \propto u^2 = \left(\frac{dx}{dt}\right)^2 \propto (af)^2 \tag{7}$$

The transferred kinetic energy will also be proportion to Eq. (7). Figure 11 represents the $(af)^2$ versus the average packing density plotted in Figs. 9 and 10. As shown in Fig. 11, the average packing density seems to be described as a function of multiplication of amplitude and frequency in the present analyses. Furthermore, one can estimate the most appropriate vibrating condition using the present pseudo 3D DEM.

In an actual fuel manufacturing, a vibro-filling process of a long fuel pin (approximately 3m) will be planned [6]. In case of the long pin vibration, a second or higher order vibration mode will appears and the optimal vibrating condition may change comparing with the short pipe configuration. Consequently, the present method will be useful and

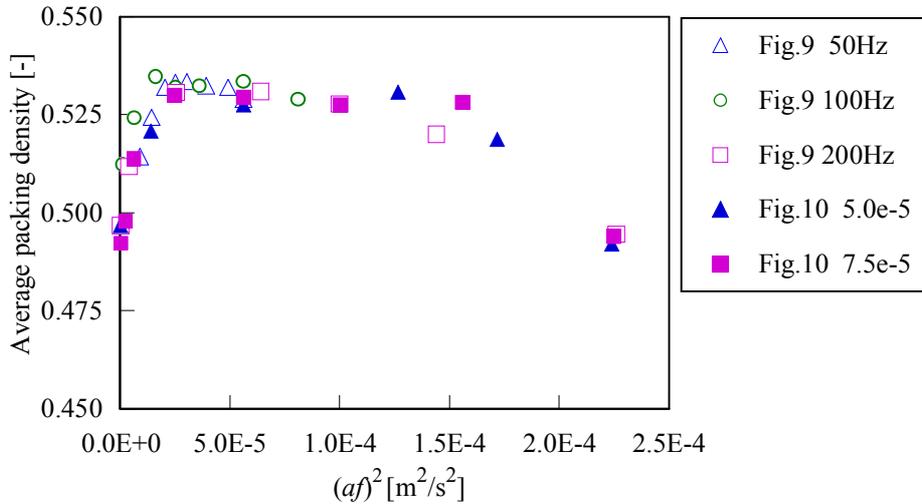helpful to understand and investigate the influence of multiple vibration mode.

Fig. 11 (af)^2 versus Packing Density (all analytical results in Figs. 9 and 10)

4. CONCLUSION

A numerical simulation of particle infiltration, which will be occurred in a viro-filling process of a low-decontaminated Mixed Oxide fuel fabrication, has been carried out using a pseudo three-dimensional (3D) Distinct Element Method (DEM). In the pseudo 3D DEM, a virtual diameter that is calculated based on an orthographic projection of three-dimension onto two-dimension is introduced in a two-dimensional DEM so as to simulate an infiltration phenomenon with low computational cost.

In the present study, sensitivity analyses of frequency and amplitude in the vibration have been carried out as well as the comparison between the pseudo 3D and 3D DEMs.

As a result of the comparison between the pseudo 3D and 3D DEMs, a good agreement of the qualitative tendency is obtained in terms of the packing density distribution along the vertical axis of the container though it is underestimated in the pseudo 3D DEM. The underestimation of the packing density comes from the simplified alignment in the present method. However, it has a great advantage that the infiltration phenomenon can be predicted with a low computational cost (approximately one tenth of the 3D DEM).

It is also concluded that the most appropriate vibrating condition will exist and be estimated using the present method. In case of a single mode vibration of simple sine curve, the packing density might be a function of the multiplication of amplitude and frequency.

A mature comparison between the pseudo 3D and 3D DEMs, such as a momentum and kinetic energy balance along to each axis, will be carried out in the future. An experimental verification and the numerical modification of the pseudo 3D DEM are also planned.

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