Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 17-18, 2018

The improvement of the prediction of solid particle sedimentation characteristic in liquid pool using the CFD-DEM algorithm

Byoungcheol Hwang, Hyun Sun Park *, and Moo Hwan Kim
Division of Advanced Nuclear Engineering, POSTECH, Hyoja-dong, Nam-gu, Pohang, Kyung-buk, South Korea
**Corresponding author: hejsunny@postech.ac.kr*

1. Introduction

When molten core, so called corium, penetrates the reactor pressure vessel in the late phase of Severe Accident, the long-term coolability of corium is important in the consideration of the integrity of reactor containment. In the case of flooding cavity, the corium interacts with the coolant, and is fragmented into solid melt particle. The analysis for the sedimentation and formation of solid melt particles is important because its overall shape and inner structure affect largely on the long-term coolability [1-2]. The numerical approach for solid particle sedimentation in liquid pool using the CFD-DEM algorithm have been performed in previous researches [3-5]. In this research, the analysis of interaction models of particle-fluid and particle-particle with consideration for drag coefficient model, type of numerical model related with pressure calculation, and rolling friction model. In the results of simulation, the reduction of particle falling time comparing with experimental data was shown, and the better prediction comparing to the previous calculation [3] for particle sedimentation phenomenon such as maximum bed height, and particle bed distribution was shown.

2. Methods and Results

2.1 CFD-DEM algorithm

The CFD-DEM algorithm is the coupled numerical scheme that the Computational Fluid Dynamics (CFD) treating the fluid regime, and the Discrete Element Method (DEM) treating the trajectory of solid particle. The advantage of this algorithm is that a number of particle-particle collision can be calculated efficiently using the simple contact model in DEM. Also the particle-fluid interaction can be considered using the concept of momentum exchange. Many industries such as food engineering, civil engineering, pharmaceutical field, and so on use the algorithm in numerical simulation. In this research, the Eulerian-based CFD that uses the locally-averaged Navier-Stokes equation, and the gird size larger than the size of a solid particle were adopted. In the interaction between fluid and solid phases, the momentum exchange is considered including several terms such as buoyancy, and drag force. The main computational algorithm of CFD-DEM is: (1) the particle information such as position and velocity is computed in the DEM solver, (2) these data are transferred to the CFD solver, and the solver calculates the volume fraction of fluid, and momentum exchange, (3) the fluid force calculated in the CFD solver is transferred to the DEM solver and the stage returns back to stage (1). The detailed explanation about the algorithm is written in the previous research [3].

2.2 Validation target of simulation for the particle sedimentation

The validation of the simulation target is conducted using the experimental data performed by Shamsuzzaman et al. in Kyushu University [6]. The purpose of the experiment is to investigate the mechanism of solid particle sedimentation phenomenon in the event of a core disruptive accident in a sodium-cooled fast reactor. The experimental facility consists of a cylindrical water pool with the diameter of 375 mm. Water is filled with up to 825 mm in height, and the funnel is set to the top of the pool (the end point of funnel is at 720 mm from the bottom). The spherical solid particles of 5L in volume are initially charged in the funnel, and the sedimentation parameters such as the particle falling time, the maximum bed height, the bed distribution are measured and analyzed. In this simulation, the cases for the nozzle size of 40 mm in diameter, the particles of 6 mm in diameters with three different materials, i.e., Al_2O_3 (3600 kg/m^3), ZrO_2 (6000 kg/m^3), Stainless steel (7800 kg/m^3), were considered. Although, this experiment is conducted with the isothermal condition, it is meaningful to validate our numerical model for the particle sedimentation phenomenon.

2.3 The consideration of simulation model and condition

In previous researches [3-6], the correlation of drag coefficient which is the function of the particle Reynolds number ($\mathrm{Re}_p = \rho v d_p/\mu$) was adopted to consider the interaction between fluid and solid phases, where ρ is the fluid density, v is the relative velocity, d_p is the particle diameter, and μ is the viscosity of fluid phase. There are a number of correlations available for the drag coefficient. Among them, the correlation by Abraham (1970) was employed in the previous simulation [3] considering the range of Re_p (Re_p< 6000) [7]. However, in the numerical simulation of particle sedimentation, the maximum velocity of a solid particle was measured larger than 1.5 m/s, meaning that the regime of Re_p is over 10^4. Therefore, the correlation by Clift and Gauvin. [8] that covers the wide range of particle Reynolds number (Re_p< 3×10^5) was applied in this research.

The types of model used in the CFD-DEM algorithm are generally classified into two approaches according to the treatment of pressure calculation [9] shown as below,

$$\frac{\partial(\rho_f \varepsilon_f u)}{\partial t} + \nabla \cdot (\rho_f \varepsilon_f u u) = -\varepsilon_f \nabla p - F_{pf}^{Model\ A} + \varepsilon_f \nabla \cdot \tau + \rho_f \varepsilon_f g \qquad \text{Eq.(1)}$$

$$\frac{\partial(\rho_f \varepsilon_f u)}{\partial t} + \nabla \cdot (\rho_f \varepsilon_f u u) = -\nabla p - F_{pf}^{Model\ B} + \nabla \cdot \tau + \rho_f \varepsilon_f g \qquad \text{Eq.(2)}$$

where, ρ_f is the fluid density, ε_f is the volume fraction of the fluid, u is the fluid velocity, t is the time, p is the pressure, F_{pf} is the particle-fluid interaction force, $\nabla \cdot \tau$ is the viscous force, and g is the gravitational acceleration. In the numerical simulation of CFD regime, if the pressure is shared by both the fluid and solid phases, it is referred to as 'model A (equation (1))', and if the pressure is attributed to the fluid phase alone, it is referred to as 'model B (equation (2))'. In that literature, the use of 'model A' was recommended because the 'model B' is appropriate only for the restricted conditions such as the steady and uniform fluid flow [9]. Therefore, the type of model was changed into 'model A' from 'model B' which was adopted in our previous calculation [4-5].

In recent numerical simulation using DEM [10], it is noted that the concept of the rolling friction is considered when the sedimentation of solid spherical particle is analyzed. According to this literature, the additional rolling friction torque was added the in the torque balance equation of solid particle to improve the prediction of the repose angle of particle lump. Therefore, the modified torque balance equation was applied in this research shown as below,

$$I_p \frac{d\omega}{dt} = r_{p,c} \times F_{p,t} + T_{p,r}\ , \qquad \text{Eq.(3)}$$

$$T_{p,r} = R_{p,\mu} k_{p,n} \Delta x_p \frac{\omega_{p,rel}}{|\omega_{p,rel}|} r_p \qquad \text{Eq.(4)}$$

where, I_p is the moment of inertia, ω the angular velocity, t is the time, $r_{p,c}$ is the particle contact radius, $F_{p,t}$ is the tangential contact force, $T_{p,r}$ is the rolling friction torque, $R_{p,\mu}$ is the rolling friction coefficient, $k_{p,n}$ is the normal spring stiffness, Δx_p is the spatial overlap, $\omega_{p,rel}$ is the relative angular velocity, and r_p is the particle radius. In these equations, the value of the rolling friction coefficient ($R_{p,\mu}$) is set to '0.1' based on the literature [10].

2.4 Simulation results on particle sedimentation phenomenon

The simulation condition is the same as the previous calculation [3] except for the drag coefficient model, type of model, and torque balance equation. Figure 1 shows the particle falling time according to density change, and the falling time in this research is defined as the period from the first particle falling out of the nozzle inlet to reaching the bottom of the catcher plate. The present calculation showed the shorter falling time for all densities than previous calculation due to the change of the drag coefficient model. When the result is compared with the experimental data, it gives an underestimated value except for the ZrO_2 (6000 kg/m^3) case. This deviation can be derived from the uncertainty of the particle-nozzle interaction in the initial stage.

The result of maximum bed height after the whole particles are settled on the bottom plate is shown in Figure 2. The previous calculation showed the underestimated values compared with experimental data, and also showed irregular behaviors as density increases. However, the present calculation in this study shows a similar behavior with the experimental data. Also, in the result of particle bed distribution of Al_2O_3 (3600 kg/m^3) particles, the high accuracy of bed distribution especially in the upper trapezoidal zone was shown in the present calculation. trapezoidal curve is shown at the side view. This change was produced from the consideration of the rolling friction.

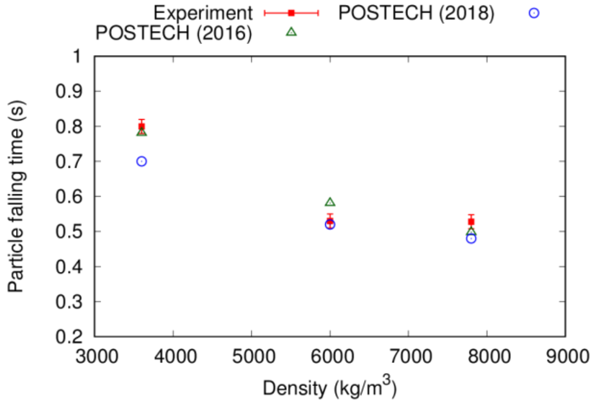

Fig. 1. Particle falling time according to density change
: Al_2O_3 (3600 kg/m^3), ZrO_2 (6000 kg/m^3), and Stainless steel (7800 kg/m^3) particles

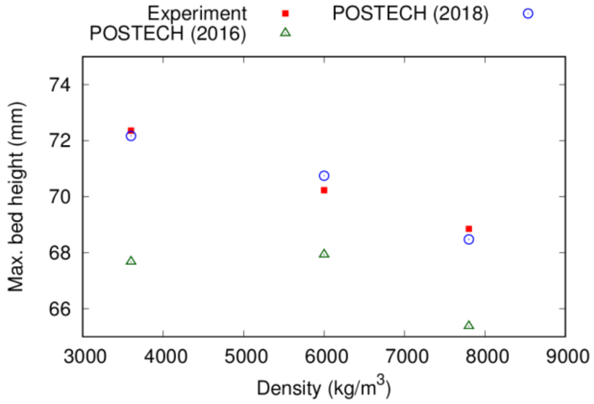

Fig. 2. Maximum bed height according to density change
: Al_2O_3 (3600 kg/m^3), ZrO_2 (6000 kg/m^3), and Stainless steel (7800 kg/m^3) particles

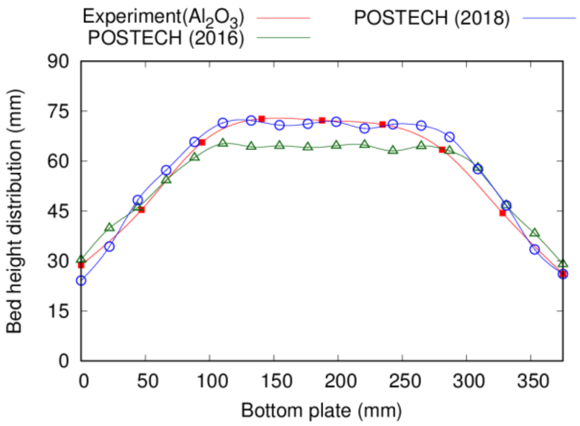

Fig. 3. Particle bed distribution of Al_2O_3 (3600 kg/m^3) particles

3. Conclusions

In order to improve the numerical simulation using the CFD-DEM algorithm for the solid particle sedimentation in liquid pool, the computational characteristic of CFD-DEM was considered. In this research, the new correlation of drag coefficient covering the broad range of particle Reynolds number, the new type of CFD-DEM model considering the both effect of fluid and solid on pressure calculation, and the addition of the rolling friction concept affecting the formation of particle cloud were adopted, and the results were compared with the previous calculation. The results show that the particle falling time was shorter than the experimental data except for the case of ZrO_2 particle, and the further consideration for the uncertainty of particle-nozzle interaction should be needed. The results of maximum bed height and particle bed distribution show the accurate simulation comparing with experimental data due to the effect of the rolling friction. In order to perform the numerical validation for particle sedimentation, the additional comparison of result parameters such as overall shape of particle bed (concave or convex), particle average velocity during the transient state of falling, and so on should be considered.

ACKNOWLEDGEMENT

This work was supported by the Nuclear Safety Research Program through the Korea Foundation Of Nuclear Safety(KOFONS), granted financial resource from the Nuclear Safety and Security Commission(NSSC), Republic of Korea (No. 1305008).

REFERENCES

[1] E. Takasuo, Debris coolability simulations with different particle materials and comparisons to COOLOCE experiments, VTT Research Report VTT, 2013.

[2] S. Thakre, and W. Ma, An experimental study on coolability of a particulate bed with radial stratification or triangular shape, Nuclear Engineering and Design, Vol.276, p.54-63, 2014.

[3] B. Hwang, and H. S. Park, Three-dimensional Two-way Coupling CFD-DEM Simulation of Particle Sedimentation in Severe Accident, Transactions of the Korean Nuclear Society Autumn Meeting, KNS, Gyeongju, Korea, Oct. 27-28, 2016.

[4] B. Hwang, W.H. Jung, Moo Hwan Kim, and Hyun Sun Park, Numerical Simulation of Debris Particle Sedimentation in Ex-vessel Severe Accident using the CFD-DEM algorithm, The 8th Korea-China Workshop on Nuclear Reactor Thermal-Hydraulics (WORTH-8), Yeosu, Korea, Oct. 22-24, 2017.

[5] B. Hwang, and H. S. Park, Analysis of particle trajectory and sedimentation characteristics under water based on the CFD-DEM algorithm, KSME2017, pp. 491-496, 2017.

[6] M. Shamsuzzaman, B. Zhang, T. Horie, F. Fuke, T. Matsumoto, K. Morita, and Y. Tobita, Numerical study on sedimentation behavior of solid particles used as simulant fuel debris. Journal of Nuclear Science and Technology, Vol.51, No.5, 681-699, 2014.

[7] F. F. Abraham, Functional dependence of drag coefficient of a sphere on Reynolds number. The Physics of Fluids, Vol.13, No.8, 2194-2195, 1970.

[8] R. Clift, and W. H. Gauvin, Proc. Chemeca ’70, Vol.1, pp.14-28, 1970.

[9] Z. Y. Zhou, S. B. Kuang, K. W. Chu, and A. B. Yu, Discrete particle simulation of particle–fluid flow: model formulations and their applicability. Journal of Fluid Mechanics, Vol.661, pp.482-510, 2010.

[10] C. Goniva, C. Kloss, G. N. Deen, A. J. Kuipers, and S. Pirker, Influence of rolling friction on single spout fluidized bed simulation. Particuology, Vol.10 No.5, pp.582-591, 2012.