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Three-dimensional Two-way Coupling CFD-DEM Simulation of Particle Sedimentation in Severe Accident

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1. Introduction

This numerical simulation is related with the accident progress in ex-vessel Severe Accident for Light Water Reactors (LWRs), or Sodium-cooled Fast Reactors (SFRs). When the molten core material penetrates the lower plenum of pressure vessel, it is settled into the cavity bottom with fragmented debris particle formation by the interaction with coolant (could be water or sodium). The formation of debris bed is a crucial factor in terms of long-term coolability because the internal and external structures of debris bed determine the inflow degree of coolant [1,2,3]. Therefore, the experimental and numerical approaches for debris particle settlement were performed in Kyushu University, and the two-dimensional one-way coupling CFD (Computational Fluid Dynamics)-DEM (Discrete Element Method) simulation was used in the numerical part [4]. However, there is some limitations for showing realization such as multi-dimensional effects. Therefore, in this research, the three-dimensional two-way coupling CFD-DEM simulation was calculated and the results are compared between experimental and numerical data [4]. The comparison shows that there is some good agreements with the experimental and numerical data. Also, the characteristics of two-way CFD-DEM algorithm and the analysis for simulation results are shown in this paper.

2. Methods and Results

In this section, the brief description for experimental and numerical approaches of Kyushu University [4] is shown. Then, the algorithm and characteristics of two-way coupling CFD-DEM simulation used in this research are described. The simulation condition and the comparison of results are also included.

2.1 Experimental and numerical approaches in Kyushu University

The test facility for particle sedimentation consists of cylindrical wall (~375 mm inner diameter) filled with water (~825 mm water level). The nozzle is immersed 105 mm below the water surface, and spherical particles are initially settled inside the nozzle by blocking the plug. When the plug is removed, then particles fall free from the nozzle to bottom surface of the cylinder. Total 24 experiments were performed with three kinds of particle type (Al_2O_3, ZrO_2, and Stainless Steel), particle diameter (2, 4, and 6 mm) and nozzle diameter (20, 30, and 40 mm). Each case was tested with uniform size particle, and the three data results were defined: 1) maximum dispersion angle, 2) falling time of first particle, 3) maximum bed height. The detailed description for above three parameters are shown in section 2.4.

Also, the numerical approach was performed using CFD-DEM simulation, the coupling method between Lagrangian based DEM which is first proposed by Cundall et al. [5] and Eulerian based CFD. In Kyushu University, the 'one-way coupling' that the solid phase is affected by fluid phase and not vice versa was considered with two-dimensional domain, so they ignore the effect of fluid convection and additional multi-dimensional effect [4]. Therefore, the extension to three dimensional system should be needed for the quantitative analysis.

2.2 Characteristics of Two-way CFD-DEM coupling

In this research, the 'two-way coupling' that one phase is affected by the other phase is implemented with three-dimensional domain. The general advantage of CFD-DEM algorithm is that it can simulate massive solid particles efficiently by simplifying the inter-particle contact. In case of two-way coupling, it can also treats the interaction between solid and fluid phases by the momentum exchange in each step shown in Fig. 1.

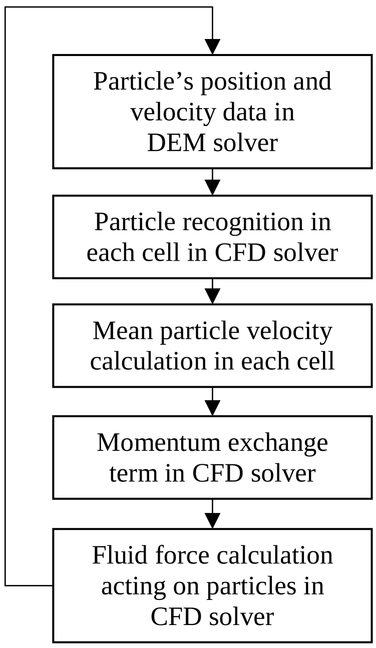

Fig. 1. Schematic diagram of two-way coupling [6]

In Lagrangian DEM approach, the force balance consists of normal, tangential, body force, and the force exerted by fluid regime is additionally considered. This force includes various kind of forces (drag force, buoyancy force, virtual mass force, Magnus force, and so on), and the only dominant two forces (drag force and buoyancy force) were considered in this research. In Eulerian CFD regime, the locally averaged Navier-Stokes equation is calculated. The momentum exchange term derived by solid particle is also calculated in the equation. More detailed information about CFD-DEM algorithm is shown in previous research [6].

2.3 Simulation condition

The material properties related with solid dynamics (Poisson ratio, coefficient of restitution, and friction coefficient) for three types of particle (Al_2O_3, ZrO_2, and Stainless steel) are shown in Table I, which are same with the data of Kyushu University [4]. Especially, there are four factors (k_n, c_n, k_t, and, c_t) consisting the inter-particle or particle-wall contact. In DEM, the contact mechanism is simplified using 'spring-dashpot concept' like Fig. 2 and Eq.(1)-(2), so the proper values of spring and damping coefficient should be considered. In this research, the stiffness related coefficients (k_n, c_n) were determined by the particle free-falling bouncing test on a solid horizontal plane, and the damping related coefficients (k_t, c_t) were calculated by considering the particle overlapping less than 1% of particle diameter [4]. Each material has different solid characteristics, so the calculated values are shown in Table I.

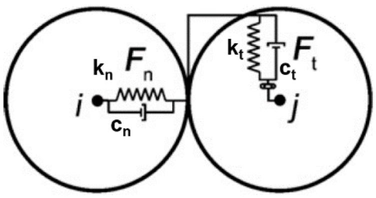

Fig. 2. Contact theory of inter-particle collision in DEM

$$F_{ij}^{n} = k_n \delta n_{ij} - c_n \frac{\delta n_{ij}}{\delta t} \quad (1)$$

$$F_{ij}^{t} = k_t \delta t_{ij} - c_t \frac{\delta t_{ij}}{\delta t} \quad (2)$$

Table I: Material properties

Material	Al_2O_3	ZrO_2	Stainless steel
Particle number	26526	26968	26305
Poisson ratio	0.27	0.27	0.27
Coefficient of restitution	0.30	0.30	0.30
Friction coefficient	0.30	0.30	0.30
k_n	89298	148830	193479
c_n	0.2558	0.4264	0.5543
k_t	35157	58595	76173
c_t	0.1007	0.1679	0.2182

The information for time step and fluid properties are shown in Table II. The time step of DEM was calculated by the Rayleigh time criteria [7], and the time step of CFD was determined by the consideration of calculation efficiency. The time step of CFD is 100 times bigger than that of DEM, because it can reduce the calculation time with having stable simulation in general [6]. Also, the property of fluid is same with the previous DEM calculations in order to analyze the accuracy of data.

Table II: Simulation condition

Parameter (unit)	Value
Time step of DEM (s)	1.0×10^{-6}
Time step of CFD (s)	1.0×10^{-4}
Fluid density (kg/m^3)	997
Fluid viscosity (N·s/m^2)	8.91×10^{-4}
Number of fluid cell	24050

In this research, CFDEM, the open-source CFD-DEM code, was used for the test calculation [8]. This code consists of LIGGGHTS (**L**AMMPS **I**mproved for **G**eneral **G**ranular and **G**ranular **H**eat **T**ransfer **S**imulations.) for DEM part [9], and OpenFOAM (**Open** source **F**ield **O**peration **A**nd **M**anipulation) for CFD part. The calculation time for each case was about 40hrs using 16 GB RAM, 4 CPU parallel processing.

2.4 Simulation Results

Fig.3 shows the particle sedimentation with transient time from 0 s to 1 s. The upper figures are the two-dimensional simulation performed by Kyushu University [4], and the lower figures are three-dimensional data results by POSTECH. The overall trends are similar, but there are small amount of particles in two-dimensional numerical data because it considers only two directions. Also, the discontinuity of particle settling can affect the flow of fluid, so the accuracy of overall bed configuration cannot be achieved. The quantitative data for comparison are maximum dispersion angle, falling time of first particle, and maximum bed height.

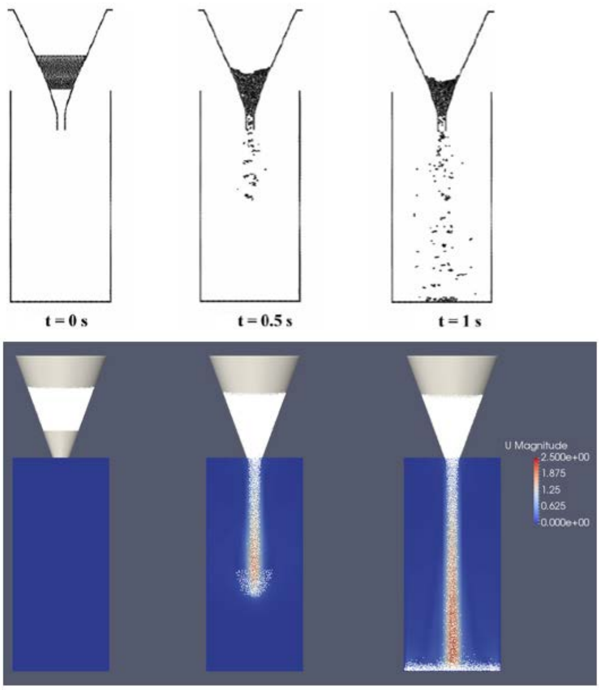

Fig. 3. Numerical data of Kyushu University [4] (upper three figures) and of POSTECH (lower three figures) with 0 s, 0.5 s and 1 s

First, the maximum dispersion angle was defined by the summation of the left and right sides maximum angle which deviated from the center line of funnel [4]. The maximum angle was shown at the early phase (~1 s) and the linear settling of particle was formed until the end of the simulation. The results of maximum dispersion angle was shown in Fig.4. The data was plotted according to the material density, and the decreasing trend of maximum angle as the density increases was shown in all experimental and numerical data. In case of stainless steel, there exists some uncertainties for measurement of maximum angle can exists because the value of three-dimensional approach was much smaller than other two data.

Fig.4 shows the particle fall time as the density of material varies. In this research, the particle fall time was calculated by measuring the time when the first particle was attached to the bottom surface. In general, the particle falling time decreases as the density of material increases, but the overall values of three-dimensional approach are higher than experimental results. This difference was caused by the initial height of particle settlement in funnel. In two-dimensional analysis, the plug barrier was considered, but no data for actual thickness of plug exists [4]. The additional geometric information for numerical simulation in Kyuhsu University should be needed for accurate validation.

The maximum bed height of debris particle bed was measured after the whole simulation was finished. In three-dimensional approach, the flow of fluid had an influence on the movement of solid particle, so the additional calculation time was needed for steady state. The difference between two-dimensional and three-dimensional analysis is large on Al_2O_3 material (~3600 kg/m^3) because of the influence of two-way coupling on the lighter density material. However, the data of three-dimensional approach is lower than two-dimensional and experimental data. This difference also affected by the initial height of particle settlement in funnel, because the previous research in Kyushu University, the height of debris bed becomes lower as the initial height of particle becomes higher [10].

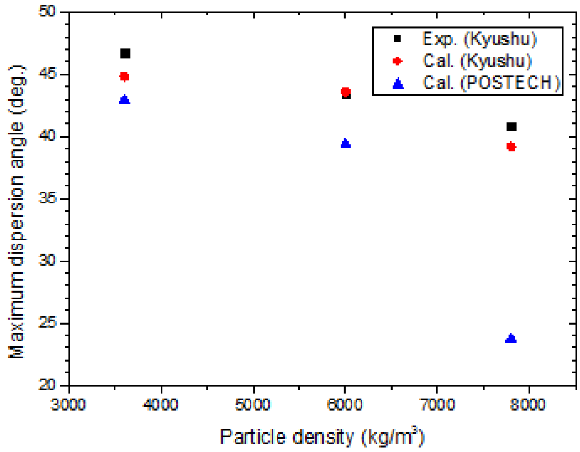

Fig. 4. Results data for maximum dispersion angle

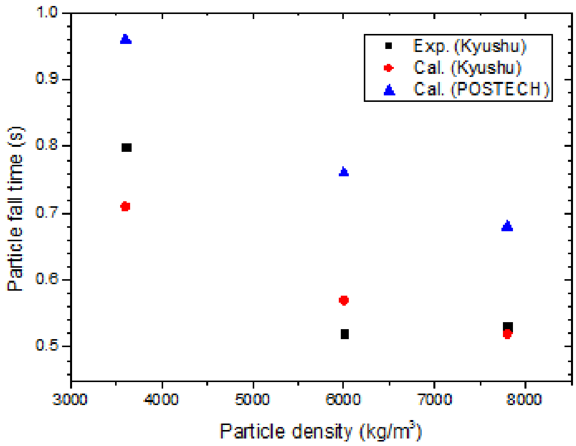

Fig. 5. Data results for falling time of first particle

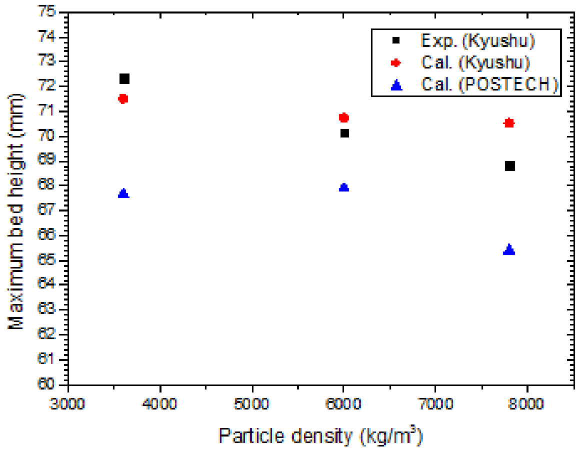

Fig.6. Data results for maximum bed height

3. Conclusions

The numerical simulation using CFD-DEM algorithm was performed in order to analyze the characteristics of debris particle bed and the realization of three-dimensional two-way coupling approach. Total three types of material (Al_2O_3, ZrO_2, and Stainless steel) were considered with fixed nozzle diameter and water level. The result parameters are maximum dispersion angle, falling time of first particle, and maximum bed height. The data for three-dimensional approach was compared with previous experimental and numerical results [4]. In maximum dispersion angle, the data except stainless steel type particle showed a good agreement. The trend of other data was similar, but the value of falling time of first particle was larger than other two cases. Also, the results of maximum bed height was lower than other two cases, and these differences were caused from the uncertainty of initial particle settlement in funnel rather than inter-particle, particle-wall interaction, and so on. In order to perform further analysis, the accurate information of previous researches should be needed, and the quantitative approach should be considered such as the distribution curve of debris bed height and the velocity of fluid.

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