Numerical Simulation of 3-Phase Debris Bed Hydrodynamic Behavior Using Multi-phase SPH-DEM Coupling

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1. Introduction

In the late phase of severe accident of reactor, there are some fluid-solid 3-phase flow issues associated with debris bed. For instance in the LWR ex-vessel cooling for the wet cavity strategy, the conical shape of particulate debris bed may be leveled due to the two-phase natural convection of the coolant (Fig. 1), which can be an important issue in terms of coolability of debris bed [1, 2]. This fluid-solid 3 phase phenomena contain transient and non-linear interface between liquid and vapor phase, and the collision interaction between particulate debris as well. Therefore, coupling Lagrangian-based multi-phase CFD techniques and discrete element method can be an effective approach to simulate the sharp and dynamic behavior of 3-phase flow involving solid particles.

In this respect, an integrated numerical code for 3D 3-phase flow has been developed in this study by two-way phase coupling of multi-phase Smoothed Particle Hydrodynamics (SPH) model and solid particle Discrete Element Method (DEM) model. 3D high-resolution simulation for the behavior of particulate debris bed has been performed through the GPU-based parallelization of the coupled SPH-DEM code.

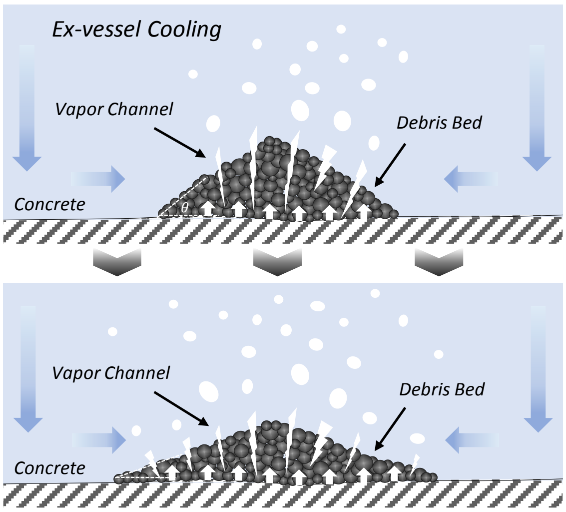

Fig. 1. Debris bed leveling behavior

2. Smoothed Particle Hydrodynamics

Smoothed Particle Hydrodynamics (SPH) is one of the best-known meshless Lagrangian CFD methods in which the fluid system is replaced by the finite number of particles that carry individual properties [3]. The SPH technique can be effectively used to simulate non-linear and sharp two-phase flows due to its Lagrangian nature of easy interface tracking. The particle approximation scheme and governing equations for multi-phase SPH method are summarized in this section.

2.1 SPH Particle Approximation

The SPH is based on an interpolation method which is basically the theory of integral interpolants using delta function.

$$f(x) = \int_{\Omega} f(x')\delta(x - x')dx' \qquad (1)$$

The variable x denotes the point in volume Ω, and δ denotes the Dirac delta function which has a value of zero everywhere except for at a certain point and whose integral over the entire region is equal to one. The discretized formulation of SPH particles can be obtained by using the kernel functions that approximate a delta function.

$$f(r_i) = \sum_j f(r_j)W(r_i - r_j, h)V_j \qquad (2)$$

The variable $f(r_i)$ is a function at the position i, subscript j represents the adjacent particles of particle i, V is the particle volume, and $W(r_i - r_j, h)$ stands for the kernel function, where h denotes influencing area of the kernel weighting function. The kernel function is a symmetric weighting function of particle distance which should be normalized over its support domain. The simplified principle of SPH approximation is described in Fig. 2.

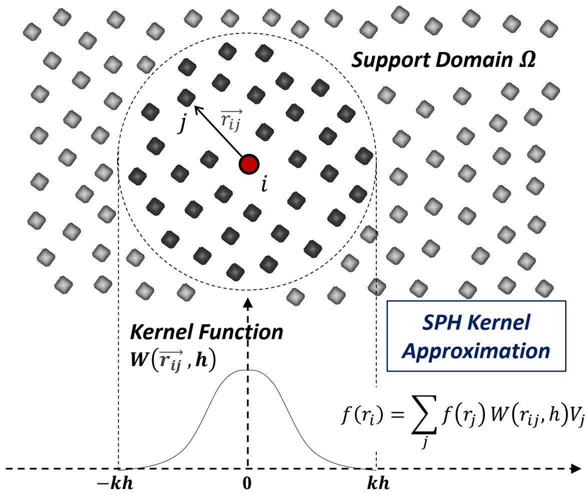

Fig. 2. SPH Particle kernel approximation

2.2 Multi-phase SPH Governing Equations

The main governing equations describing the motion of an isothermal, Newtonian viscous fluid within incompressible flow condition are the mass conservation and the Navier-Stokes equations (momentum equation). In the general SPH approach, a slight fluctuation in density is allowed also for the incompressible fluid, and the pressure is explicitly calculated from the equation of state as a function of density. The SPH formulations for governing equations are summarized in Table I.

In order to accurately handle the two-phase interface with high density ratio, the density of fluid particles for each phase is estimated based on the normalized density (eqn (3)), and each term of the N-S equation is discretized in volume-based SPH formulation (eqn (4), (5)). In addition, Continuum Surface Force (CSF) model (eqn (6)) and interface sharpness force are employed in order to treat the surface tension at the interface between each phase.

Table I. SPH formulations for governing equations

Density Estimation : Normalized Density [4]	
$\rho_i = \rho_{ref,i} \sum_j \frac{m_j}{(\rho_{ref})_j} W_{ij}$	(3)
Momentum Conservation (Navier-Stokes Equation) [5, 6]	
$\left(\frac{d\vec{u}}{dt}\right)_{fp,i} = -\sum_j m_j \left(\frac{p_i + p_j}{\rho_i \rho_j}\right) \nabla W_{ij}$	(4)
$\left(\frac{d\vec{u}}{dt}\right)_{fv,i} = \sum_j \frac{4 m_j \mu_j \, \vec{r_{ij}} \cdot \nabla_i W_{ij}}{(\rho_i + \rho_j)\left(\lvert\vec{r_{ij}}\rvert^2 + \eta^2\right)} (\vec{u_i} - \vec{u_j})$	(5)
$\left(\frac{d\vec{u}}{dt}\right)_{fs,i} = \frac{\sigma_i}{\rho_i}\left(dim \frac{\sum_j (\hat{n_i} - \varphi_i{}^j \hat{n_j}) \nabla W_{ij} V_j}{\sum_j \lvert r_i - r_j \rvert \lvert \nabla W_{ij} \rvert V_j}\right) \vec{n_i}$	(6)
Equation of State [7]	
$p_i = \frac{{c_{0i}}^2 \rho_{0i}}{\gamma} \left[\left(\frac{\rho_i}{\rho_{0i}}\right)^\gamma - 1\right]$	(7)

3. Discrete Element Method

Discrete Element Method (DEM) is one of a direct simulation method for a rigid body that can analyze the transition, rotation, and collision behavior of solid particles in detail based on Newton's law of motion [8]. The basic concept and contact force model for DEM method are summarized in this section

3.1 Concept of DEM Rigid Body Method

In the DEM method, the collision and following transition and rotation of each rigid body are directly solved in detail. In the general DEM method, the collision between rigid bodies is solved in spring-dashpot model (Fig. 3) based on the soft-sphere approach. The spring, damper, and slider in Fig. 3 represent the elastic term, energy dissipation term, and friction force term in the collision between two particles respectively.

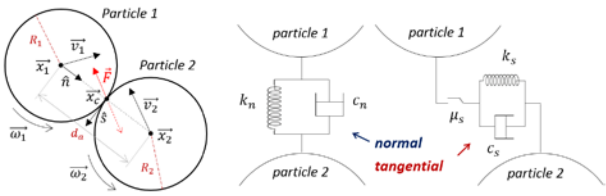

Fig. 3. Soft-sphere spring-dashpot collision model

3.2 DEM Contact Force Model

Based on the above spring-dashpot collision model, the contact force between two particles in normal and tangential direction consists of elastic term and damping term while the tangential force is determined through an additional comparison with the frictional force.

$$\vec{f_c} = (k_n \delta_n - c_n \lvert\vec{v_{cn}}\rvert)\hat{n} + f_s \, \hat{s} \qquad (8)$$

$$f_s = \min\left(k_s \delta_s - c_s \lvert\vec{v_{cs}}\rvert \, , \, f_{friction}\right) \qquad (9)$$

The subscript n and s represents the normal and tangential direction in the collision, and the variable k and c denotes the spring stiffness and damping coefficient between two rigid bodies. Also, the variable δ stands for the overlap between particles at the moment of collision, while $\vec{v_c}$ is the relative velocity vector between particles at the contact point. In this study, the Hertz-Mindlin contact force model is applied for the analysis of particulate system, which is summarized in Table I [9].

Table II. Hertz-Mindlin contact force model [9]

Normal Contact Force	
$k_n = \frac{4}{3} E^* \sqrt{R^* \delta_n} \qquad c_n = \sqrt{\frac{10}{3}} \frac{\ln(e)}{\sqrt{ln(e)^2 + \pi^2}} \sqrt{M^* K'_n}$	(10)
Tangential Contact Force	
$k_s = 8 G^* \sqrt{R^* \delta_n} \qquad c_s = \sqrt{\frac{10}{3}} \frac{ln(e)}{\sqrt{ln(e)^2 + \pi^2}} \sqrt{M^* k_s}$	(11)

3.3 DEM Wall Boundary Treatment

In the general DEM technique, the interaction with the wall boundary is treated as a collision. In the case of debris bed however, the solid debris particles at the bottom may roll or slide on the wall boundary (concrete) since the heavier debris particles are packed on the bottom surface. In this respect, a versatile wall boundary condition that includes rolling and sliding behavior of the rigid body is newly proposed (Fig. 4).

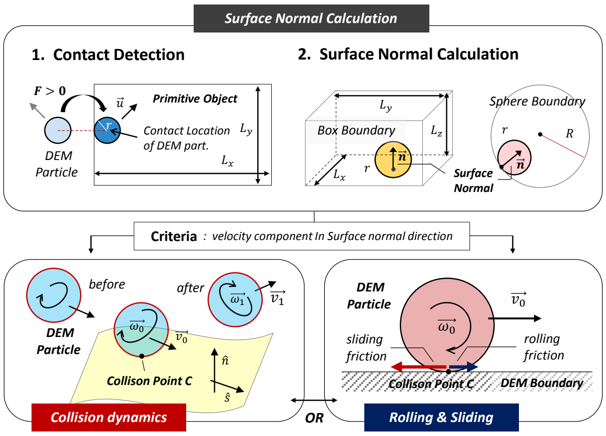

Fig. 4. New DEM wall boundary treatment model

4. SPH-DEM Two-way Phase Coupling

The numerical system for 3D 3-phase flow system is newly developed by two-way phase coupling of multi-phase SPH model and solid particle DEM model.

4.1 Unresolved Coupling of SPH-DEM

In this research, the unresolved coupling approach which allows the overlap between SPH-DEM particles was adopted considering the size of the debris particles as shown in Fig. 5. The fluid equations for the SPH particles are solved based on the local porosity within coupling domain, and the dominant forces acting on the DEM solid particles are estimated from the information of the adjacent SPH particles [10]. In addition, the interaction force acting on the SPH particles is also calculated by the Newton's third law of motion. The governing equations for SPH-DEM interaction are summarized in Table IIII where the subscript i, j denotes the SPH particle and a, b denotes the DEM particle.

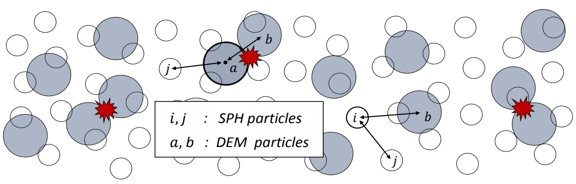

Fig. 5. Concept of SPH-DEM unresolved coupling

Table IV. Governing equations for SPH-DEM coupling

DEM Particles (buoyancy force, drag force) [10]	
$\vec{F_b} = \sum_i \frac{m_j}{\rho_j} \theta_j W_{aj} \Big/ \sum_i \frac{m_j}{\rho_j} W_{aj}$	(12)
$\vec{F_d} = \frac{1}{8} C_d \rho_f \pi d^2 \left\lvert \vec{u_{ja}} \right\rvert \vec{u_{ja}} \varepsilon^{2-\chi}$	(13)
SPH Particles (Newton's third law of motion)	
$\left(\frac{du}{dt}\right)_i = -\sum_i m_j \left[\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right] \nabla_i W_{ij} + S_i + \vec{g}$ $S_i = -\frac{1}{\rho_i} \sum_b \frac{1}{\sum_j \frac{m_j}{\rho_j} W_{bj}} \vec{F_b} W_{ib}$	(14)

4.2 Algorithm of Coupled SPH-DEM Model

The SPH and DEM are both explicit Lagrangian based numerical simulation techniques. Thus, the time-step limitation of the SPH calculation is similar to that required in DEM simulation especially when considering the vapor phase in SPH. For this reason, the phase coupling of SPH-DEM model is performed within the single algorithm as shown in Fig. 6. Neighboring particles searching (NNPS) for SPH particles and contact detection for DEM particles are independently carried out based on each cell size.

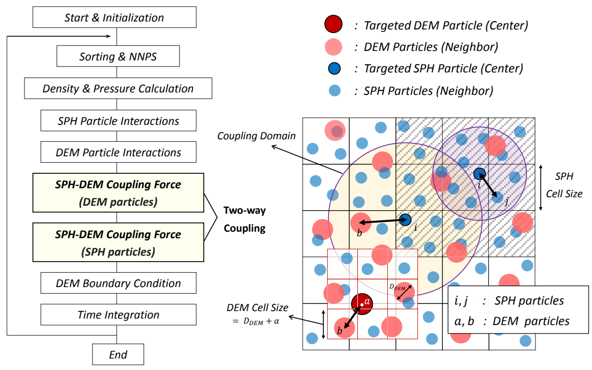

Fig. 6. Simplified algorithm of SPH-DEM phase coupling

4.3 Validation of Coupled SPH-DEM Model

The validation of SPH-DEM phase coupled model has been carried out through the terminal velocity behavior and the 3D dam-breaking behavior. In the former case (Fig. 7), the velocity over time was compared with the analytic solution where the same drag coefficient correlation was applied, and the dependence on the size of the coupling domain was analyzed. In the dam-break simulation (Fig. 8), the position of the water front over time was compared with the benchmark experiment data.

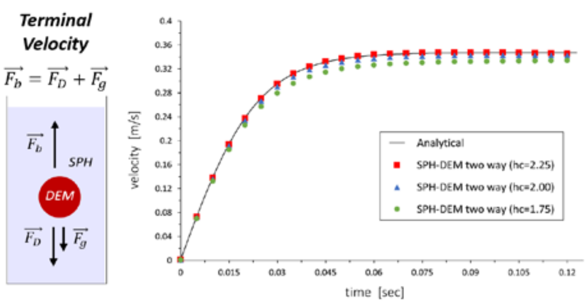

Fig. 7. Terminal velocity behavior of single DEM particle

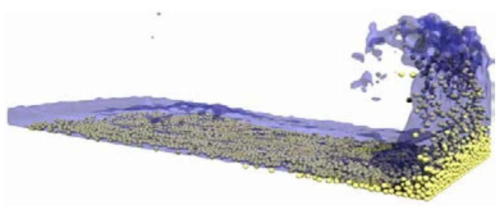

Fig. 8. 3D dam-break simulation of SPH-DEM coupled model

5. GPU Parallelization of Coupled SPH-DEM Code

The SPH-DEM coupled model developed in this study is parallelized through NVIDIA's CUDA architecture. Parallel mapping and reduction are applied for solving discretized summation equations of each SPH particle, solving contact force equations of each DEM particle, and also solving coupling equations between SPH-DEM particles. In addition, particle searching (NNPS) for SPH and contact detection for DEM are also accelerated through the various parallelization algorithms.

6. 3D Simulation of Debris Bed Behavior

The 3D simulations has been conducted for possible hydrodynamic behavior of debris bed in reactor accident conditions using SPH-DEM phase coupled model. The vapor driven 3-phase leveling behavior of solid debris particles, which can be occurred in the ex-vessel cooling condition in LWR, is also simulated as shown in Fig. 9 and Fig. 10. The results show good agreement with the benchmark experiment both in qualitative and quantitative manners.

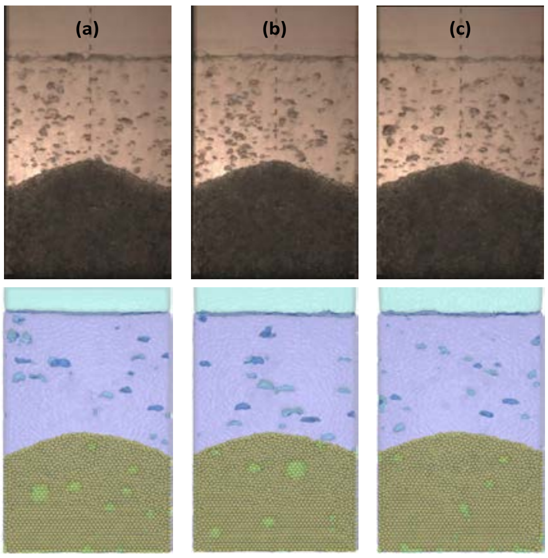

Fig. 9. Results of vapor-driven self-leveling simulation

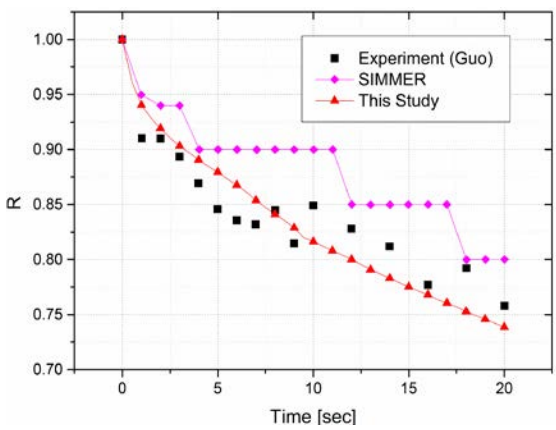

Fig. 10. Validation results for time variation of inclined angle

7. SUMMARY

In this study, the SPH-DEM phase coupled numerical model is developed for the simulation of dynamic 3-phase phenomena involving solid particles such as liquid sloshing and vapor induced debris bed self-leveling. The two-way phase coupling of SPH and DEM models is conducted in unresolved manner after implementing the both models individually. In addition, the GPU-based parallelization of developed SPH-DEM code is performed in order to retain capability of 3D high resolution simulations. Finally, the 3D simulations for centralized sloshing and vapor induced particle leveling behavior is carried out and validated.

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