Numerical Simulation on LMR Molten-Core Sloshing Behaviors Using Smoothed Particle Hydrodynamics Method

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1. Introduction

In transient phase of core disruptive accident of liquid metal reactor, a neutronically active multiphase pool can be formed which is composed of solid fuel, molten fuel, re-frozen fuel, fission gas, fuel vapor, steel particles, and so on. In this configuration, abrupt pressure build-up due to the local vapor generation can initiate so-called centralized sloshing motion (Fig.1) which has a potential for energetic re-criticalities of fuel[1,2].

In this study, 3D two-phase sloshing motion has been simulated using GPU parallelized in-house SPH code in order to identify the difference in presence of the vapor phase. Maximum sloshing height and time in each condition are validated through the comparison with benchmark experiments and analytic studies. Also, the results of the simulation are analyzed in various aspects such as the particle resolution, and the effect of vapor phase.



Fig. 1. Centralized Sloshing Behavior of LMR Pool [2]

2. SPH Method

2.1 Concept of SPH method

SPH is a meshless Lagrangian method developed in 1977[3] for astrophysical area. In the SPH method, the fluid system is represented by a finite number of particles that carry individual properties, and the governing equations of each particle are solved in discretized smoothing formulation over the neighboring particles. The SPH method exhibits large advantages come from its Lagrangian nature in dealing with free surface flow, highly deformable geometry, multiphase flow, and so on. Also, the convective term in governing equation is naturally reflected in the standard SPH formulism without solving any nonlinear matrix, so the convective flow and convective heat transfer can be implemented without any difficulty. In addition, it is relatively easy to implement a wide range of physical models with standard SPH method, since it solves quasiincompressible equation of state instead of solving the pressure Poisson equation.

2.2 SPH Particle Approximation

The SPH approximation is based on an interpolation method which is basically the theory of integral interpolants using delta function. The discretized formulation of SPH particles can be obtained by using the kernel functions that approximate a delta function.

$$f_i(r) = \sum_i f_i W(r_i - r_j, h) V_j \tag{1}$$

The variable f_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.



2.3 SPH Governing Equations

In the SPH method, the main governing equations are solved in Lagrangian frame.

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{u} \tag{2}$$

$$\rho \frac{\vec{du}}{dt} = -\nabla p + \mu \nabla^2 \vec{u} + \rho \vec{g} \tag{3}$$

where ρ and \vec{u} are the density and velocity of the fluid, p, μ and g denote pressure, dynamic viscosity, and the gravitational constant, respectively. The discretized SPH equations of the continuity equation (2) and each term of momentum equation (3) can be derived in various form according to the integral method and interaction strategies between particles. The SPH formulations of each RHS term in the above equation (2) and (3) are summarized in Table I including density diffusion model (δ -SPH). For the equation of state, Tait equation is generally used for SPH which assumes the incompressible fluid as a weakly compressible fluid, allowing the slight compressibility of the fluid.

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Table I	NPH.	tormulations	tor	governing	equiptions
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Governing Eq	SPH formulation	
Mass Conservation	$\left(\frac{d\rho}{dt}\right)_{i} = \rho_{i} \sum_{j} \frac{m_{j}}{\rho_{j}} \left(\overrightarrow{u_{i}} \cdot \overrightarrow{u_{j}}\right) \cdot \bigtriangledown_{i} W_{ij}$	
(Density Diffusion)	$\left(\frac{d\rho}{dt}\right)_{i} = 2\delta hc_{0}\sum_{j}\psi_{ij}\left(\frac{m_{j}}{\rho_{j}}\right) \frac{\vec{r_{ij}}\cdot\nabla_{i}W_{ij}}{\left \vec{r_{ij}}\right ^{2}}$	
Momentum Conservation	$\left(\overline{ \frac{d u}{d t}} \right)_{fp,\ i} = -\sum_j m_j \left(\frac{p_i + p_j}{\rho_i \rho_j} \right) \bigtriangledown W_{ij}$	
	$\left(\frac{\overrightarrow{du}}{dt} \right)_{\text{fv},i} = \sum_{j} \frac{4m_{j}\mu_{j} \overrightarrow{r_{ij}} \cdot \bigtriangledown_{i} W_{ij}}{\left(\rho_{i} + \rho_{j}\right) \left(\left \overrightarrow{r_{ij}} \right ^{2} + \eta^{2} \right)} \left(\overrightarrow{u_{i}} \cdot \overrightarrow{u_{j}} \right)$	
	$\left(\overline{ \frac{\mathrm{d} u}{\mathrm{d} t}} \right)_{\mathrm{fva},i} = \sum_j m_j \Pi_{ij} \bigtriangledown_i W_{ij}$	
Equation of State	$p = \frac{c_0^2 \rho_0}{\gamma} \left[\left(\frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right]$	

3. Implementation of In-house SPH solver

3.1 SOPHIA Code

The SOPHIA code is a GPU-parallelized SPH solver under development in Seoul National University (SNU) for complicated multi physics application associated with nuclear reactor safety. It currently incorporates basic conservation equations summarized in Table I, and various physics including heat transfer, turbulence, multi-phase, mass diffusion, elastic solid, and so on. In addition, the numerical methods such as density renormalization and correction filters are applied to guarantee the second order accuracy for the whole computational domain. All the detailed function of SOPHIA code is fully parallelized by CUDA GPU architectures for performance improvement. Fig. 3 shows the simplified system of SOPHIA solver.

3.2 Normalized Density Formulation

The general SPH density estimation method in Table I can generate unphysical density and pressure near the interface between the fluids with different density. This problem is originated from the discontinuous density field in multi-fluid or multi-phase flow. To handle the



Fig. 3. Simplified System of SOPHIA Solver

two-phase simulation with high density ratio, the normalized density, which is a continuous function on the interface, is suggested as the primary variable for density calculation in this study. This new approach estimates the normalized density instead of density so that it can prevent the generation of unphysical pressure near the interface even in two-phase simulation. The final equation after the derivation is as follows.

$$\frac{d}{dt} \left(\frac{\rho}{\rho_0}\right)_i = -\left(\frac{\rho_i}{\rho_{0,i}}\right) \sum_j V_j \left(\overrightarrow{u_i} - \overrightarrow{u_j}\right) \cdot \nabla W_{ij} \qquad (4)$$

$$\left(\frac{\rho}{\rho_0}\right)_i = \sum_j \frac{m_j}{\rho_{0,j}} W_{ij} \tag{5}$$

3.2 GPU-based Parallelization

The SOPHIA code adapts CUDA GPU architectures for parallelization and performance improvement. The Tesla P100 device is used as an acceleration device, and all the SOPHIA functions and detailed algorithms including nearest neighboring particles searching (NNPS) are fully parallelized. Based on benchmark calculations, the parallelized code shows much higher performance by two orders of magnitude compared to the single CPU code for 1.0 million particles as shown in Fig. 4. In detail, the parallelization factor is calculated over 0.99 in case of a million particles, which is enough to expect a sufficient performance improvement by parallelization. Also, it can be said that the GPU parallelization is efficient enough since the speedup factor for Tesla P100 cores reaches more than 97% of the convergence value.



4. SPH Simulation of Centralized Sloshing

4.1. Geometry and Conditions

In this study, experimental results of Maschek[4] were selected as benchmark data for code validation. The experiments were composed of 5 series according to the geometry and conditions including various type of disturbances. In this study, three out of five experimental conditions are selected to simulate 3 dimensional single/two phase sloshing behavior. The initial condition and geometry for each case is shown in Fig.5.



Fig. 5. Geometry for 3D SPH Sloshing Simulation

4.2. Qualitative SPH Result of 3D Sloshing

4.2.1. Case 1 Centralized Sloshing (Single-phase)

In the high resolution SPH simulation, 3,621,592 particles are participated. The snapshots of simulation in are arranged in Fig. 6. Compared with the benchmarking experiment, SPH code in this study well simulates this series of liquid sloshing behavior as shown in Fig. 7.



Fig. 6.3D Single-phase SPH Simulation for Case 1



(a) 0.0 [sec] (b) 0.1 [sec] (c) 0.4 [sec] (d) 0.6 [sec] (e) 0.865 [sec] Fig. 7. Qualitative Comparison of SPH Results with Exp

4.2.2. Case 2 Vertical Rods (Single-phase)

The 3D SPH simulation for 12 vertical inner/outer rods are carried out in same particle resolution compared with the above centralized sloshing. The snapshots for each rod condition is shown in Fig. 8. The SPH result in this study well describe the damping and interference motion of water waves by rod disturbances.



Fig. 8. 3D Single-phase SPH Simulation for Case 2

4.2.3. Case 3 Asymmetric Sloshing (Single-phase)

If the initial water column is asymmetrically located, different traveling distance of water wave prevents large local accumulation of water. Therefore, central sloshing behavior do not develop, rather moves chaotically in the container in this configuration (Fig. 9)



Fig. 9. 5D Single-phase SPH Simulation for Case 5

4.2.4. Case 1 Centralized Sloshing (Two-phase)

The 3D SPH simulation for two-phase condition has been conducted applying the novel normalized density estimation method proposed in this study. Around 10 million particles were used in simulation including air particles, and the result is shown in Fig. 10. Overall behavior including sloshing height and time was not significantly different with single-phase simulations.



Fig. 10. 3D Two-phase SPH Simulation for Case 1

4.3. Validation Results for SPH Sloshing Simulation

The maximum sloshing height and time for each case are compared with benchmarking experiments and other analytic studies. Most of the results are in a good agreement with experiments especially for the high resolution and two-phase simulation (Table I).

Table II. Validation of SPH Results with Experiment						
Slosh at pool center	Times[s]	H [cm]				
Case 1. Centralized Sloshing						
Experiment [4]	0.88	40.0				
SIMMER [5]	-	>50				
SPH [6]	0.87	38.0				
SOPHIA - high resolution	0.88	38.0				
SOPHIA - low resolution	0.86	36.3				
SOPHIA - two-phase, med	0.87	41.0				
Case 2. Vertical Rods Sloshing (Inner/Outer)						
Experiment [4]	0.90	3.0				
SPH [6]	0.82	5.0				
SOPHIA	0.88	3.5				
Experiment [4]	0.88	15.0				
SPH [6]	0.84	15.5				
SOPHIA	0.88	12.9				
Case 3. Asymmetric Sloshing						
Experiment [4]	0.48	24.0				
SIMMER [5]	0.48	21.0				
SOPHIA	0.47	21.0				

4.4. Discussions of SPH Results

4.4.1. Effect of Particle Resolution

The SPH simulation results are highly affected by the particle resolution in sloshing phenomena as summarized in Table III. Generally, the lower resolution makes the lower number density of particles in center sloshing motion, finally resulting in a generation of fragmented particles and dampened bulk flow of piling up motion. Thus, sufficient high resolution is required for analysis of sloshing motion. As a result of parametric study for particle resolution, the maximum sloshing height in SPH simulation converges to certain value as the particle resolution increases as shown in Fig.11

4.4.2. Effect of Vapor Phase in SPH Simulation

The maximum sloshing of two-phase SPH simulation is closest to benchmark experiment value as summarized in Table II. In two-phase simulation, there are sufficient



Fig. 11. Effect of Particle Resolution in SPH Result

particles (including air particles) in the support domain regardless of the particle resolution in sloshing peak, while particle deficiency may occur in single phase simulation. As a result of particle deficiency, unphysical high-speed stream of solitary particles can be created as shown in 2D results in Fig. 12. Similarly, the behavior near gas trapping area may differ each other due to the same issue. Since this small difference can be amplified as a large disturbance of wave, the precise analysis based on two-phase model is required for sloshing behavior.



Fig. 12. Comparison between Single and Two Phase Results

5. Summary

In this study, the single/two phase sloshing behavior is simulated using 3D GPU parallelized SPH solver with a novel normalized density estimation method. The results of SPH simulations show good agreement with the benchmark experiment both in qualitative and quantitative manners, especially for the high resolution simulation. Also, it has been identified that the two-phase SPH simulation best predicts the sloshing height since it can prevent the local numerical errors from particle deficiency in sloshing peak and gas trapping motions.

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