Transactions of the Korean Nuclear Society Virtual Spring Meeting
July 9-10, 2020

Coupling of Particle-based Simulation and MARS Code for Simulation of IVR-ERVC: Preliminary Study

So-Hyun Park [a], Hoon Chae [a], Eung Soo Kim [a*], Chang Won Lee [a], Hyoung Kyu Cho [a], Yeon-Gun Lee [b], Min Seop Song [a]

[a]*Dept. of Nuclear Engineering, Seoul Nat'l. Univ., 1 Gwanak-ro, Gwanak-gu, Seoul, Korea*
[b]*Dept. of Nuclear and Energy Engineering, Jeju Nat'l. Univ., 102, Jejudaehak-ro, Jeju-si, Jeju-do, Korea*

[*]*Corresponding author: kes7741@snu.ac.kr*

1. Introduction

In-Vessel Retention (IVR) through the External Reactor Vessel cooling (ERVC) is a major severe accident mitigation strategy to confine the core melt inside the lower head of the reactor vessel during the late process of core damage [1, 2]. The essence of the IVR-ERVC is to stably and sustainably remove the thermal load of the core melt trapped inside the vessel by transferring to the external coolant. In this regard, the heat transfer mechanism of the corium pool is the most important consideration because it determines the safety criterion of the reactor vessel by evaluating thermal margin to Critical Heat Flux (CHF) [2]. The thermal load that the corium pool exerts on the reactor vessel is influenced by various factors such as the thermal and hydrodynamic behavior of the corium, the heat removal rate on the outer vessel wall, and the composition and chemical behavior of the corium. In addition, the stratification/mixing of the oxide-metallic corium pool or crust formation affects the heat transfer mechanism of the corium pool [1].

To understand the complicated in-vessel corium behavior and evaluate the applicability of plant scale reactors, many benchmark experiments have been conducted, but the results are rarely applied to the safety assessment of real scale accident due to the limitation of scalability and materials [1]. Currently, based on these experimental results, several studies have developed numerical models or correlations and they have been applied to plant safety analysis. These numerical methods are mainly based on the fixed grid-based method (e.g. FVM, FEM, and FDM). Due to the nature of Eulerian based method, they suffered from handling non-confined domain such as natural convection with free surface, large interfacial deformation of stratified fluids, local phase change, and etc. This drawback has been addressed by the restrict assumptions on the complicated geometry or boundary conditions.

In this sense, this study develops the integrated code platform of the SOPHIA code (Lagrangian-based Smoothed Particle Hydrodynamics (SPH) code), and MARS code (Reactor-scale system code) in order to reduce the assumptions and uncertainties of the previous methods. The SPH method, a representative Lagrangian particle-based CFD method, analyzes the flow motion following the fluid mass point instead of a fixed lattice. Thus, the fluid system is discretized into a collection of Lagrangian particles carrying the physical properties and each particle moves according to the governing equations (mass, momentum, and energy) derived from the kernel-weighted summation over nearby particles. Because of the moving particles, the SPH method enables to effectively handle free surface or multiphase/multi-fluid flow by tracking the trajectories of fluid interfaces [3].

Using the SPH method, Seoul National University has developed the multi-dimensional and multi-physics CFD code, called 'SOPHIA' since 2015 in order to simulate the nuclear safety-related phenomena [4]. The SOPHIA code is based on the Weakly Compressible SPH (WCSPH) method that allows a slight compressibility of the fluid using equation of state (EOS). On this basis, various SPH-formulated physical models are implemented to deal with complicated phenomena; viscous force, surface tension, heat conduction, diffusion, elastic solid mechanics, etc. Since these governing equations and physical models are expressed linearly and solved by serial calculations, GPU-based parallelization becomes optimal to the SPH method. Therefore, recently, the SOPHIA code was parallelized using the multiple GPUs and it achieved dramatic improvement of the computational performance [4, 7].

However, since the SOPHIA code is a CFD-scale code, integral simulation on the IVR-ERVC phenomena encounters physical and computational limitation. For effective and efficient simulation, IVR-ERVC needs to be dealt with separately; The SOPHIA code analyzes the complicated and detailed behavior of in-vessel corium, and MARS code analyzes the external vessel cooling system.

This study aims to develop an integrated code system that couple SOPHIA code to MARS code in order to simulate the IVR phenomena more realistically and provide the best estimate of the safety analysis. For demonstrating its capability, this study performed preliminary simulation on the benchmark case that show the phenomenological characteristics of IVR-ERVC phenomena.

2. Methodology

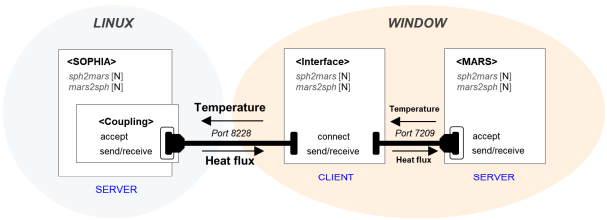
This section briefly describes the SOPHIA-MARS coupling method and the calculation procedure of each code. The codes coupling is divided into three parts:

- SOPHIA-MARS data transferring
- Analysis of external vessel cooling and circulation using MARS code
- Analysis of in-vessel corium behavior using SOPHIA code

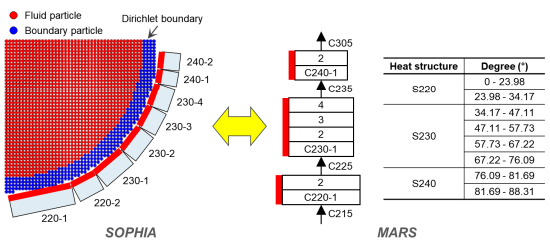
The last part of the section describes the preliminary simulation model and simulation conditions.

2.1 SOPHIA-MARS Coupling

SOPHIA-MARS code coupling is implemented using socket programming. Figure 1.(a) shows the two codes linked by socket programming. The socket performs data transmission between physically separated processes through an Internet network. As shown in figure, SOPHIA and MARS send/receive the data with interface between them. The Interface playing a role of a bridge that connects server sockets, receives the data from SOPHIA /sends to MARS and vice versa. This structure has an advantage of minimizing the modification of each server code. The exchanging data are (1) the heat flux of the inner vessel wall and (2) the temperature of the inner vessel wall. Figure 1.(b) shows the linkage of data exchange. The SOPHIA analyzes the in-vessel behavior of the core melt pool and calculates the inner wall heat flux. Taking heat flux data as an input, the MARS analyzes the external vessel cooling system. Among the calculation results of the MARS, the inner wall temperature is provided as Dirichlet boundary condition to the SOPHIA. Iterating such data transmission every time step allows to cover the entire reactor system.



(a) SOPHIA-Interface-MARS connection



(b) SOPHIA-MARS data exchange configuration

Fig. 1. SOPHIA-MARS code coupling configuration.

2.2 MARS Calculation

As mentioned before, the MARS code computes the natural circulation system between the reactor vessel and the reactor cavity. Figure 2 shows the node configuration of the MARS code. The heat structures of node no.220~240 simulate the heat load from the corium as the reactor vessel plates with 16.51cm thickness. One side boundary of the heat structure is given the heat flux as boundary condition and the other side is connected to the coolant channel. The rest nodes are as follows:

- No.120: the lower part of reactor cavity
- No.210~320: the annular channel between the reactor vessel and the insulator
- No.410~510: the annular channel between the insulator and the reactor cavity
- No.330 and 520: the free volume of the containment building

During the external vessel cooling, the coolant temperature increases along the vessel wall then the coolant circulate through the annular path due to the natural convection. If the coolant starts the nucleate boiling, the two-phase mixture of water and steam may circulate the same path as in single phase and the steam may release to the containment.

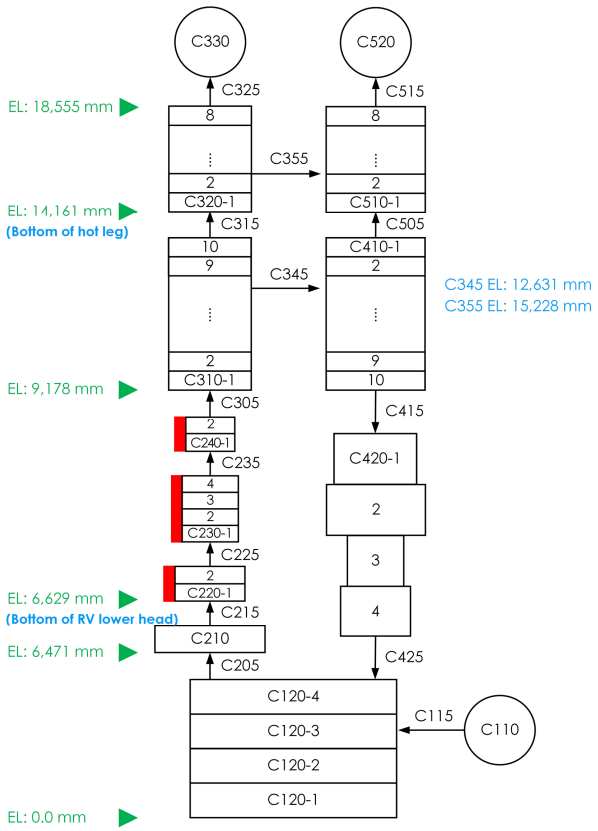


Fig. 2. MARS code node configuration.

2.3 SOPHIA Code

The SOPHIA code is developed based on the SPH method. This section briefly explain the basic concept of SPH method and the physical models implemented in the SOPHIA code. Furthermore, the new natural convection modeling enables to handle multiphase/multi-fluids system beyond the Boussinesq approximation. The way of coupling with MARS code is described in this section.

2.3.1 Fundamentals of SOPHIA

The SPH method approximates the integral of the Dirac delta function to particle summation using Gaussian-shaped weighting function and discretized finite domain particles [3]. The weighting function is referred as Smoothing kernel and the finite domain is bounded by Smoothing length. This SPH formulation can approximate a scalar/vector distribution over the space, but also approximate differential form of them. The following equations basic SPH particle-based approximation for the scalar f and its gradient respectively [3].

$$f(\boldsymbol{r}_i) = \sum_j f_j W(\boldsymbol{r}_i - \boldsymbol{r}_j, h)\frac{m_j}{\rho_j} \quad (1)$$

$$\nabla f(\boldsymbol{r}_i) = \sum_j f_j \frac{m_j}{\rho_j} \nabla W(\boldsymbol{r}_i - \boldsymbol{r}_j, h) \quad (2)$$

where $m, \rho, \boldsymbol{r}, and\ h$ denote the particle mass, density, position vector, and smoothing length. The subscript $i\ and\ j$ denote center particle and neighbor particle, respectively. W in the equation presents the smoothing kernel. In this study Wendland C2 kernel was applied [5]. On basis of above SPH formulations, the governing equations and physical models are constructed. Table 1 presents the SPH-formulated governing equations which are implemented in SOPHIA code [4]. The mass conservation is satisfied by mass summation (Eq. (3)) or continuity equation (Eq. (4)). These equations are newly formulated for multiphase/multi-fluid flow, allowing accurate density estimation in the large density gradient [6]. The momentum conservation can be decomposed into various force terms (Eq. (5)), allowing to add supplementary force terms straightforwardly. The energy conservation is simply expressed by the conduction equation (Eq.(8)) because the convection is inherently resolved by particle motion. Finally, the governing equations are closed by Equation of State (EOS). For a detailed description, refer to [4].

2.3.2 Non-Boussinesq natural convection modeling

The in-vessel corium behavior generally involves the large density gradient due to a wide range of temperature differences. This density gradient causes the convective flow, which has the significant effect on the overall heat distribution. In addition, the density difference between the oxide and metal core melt adds the complexity on the density distribution (e.g. stratification/mixing). Such a large density-gradient-driven flow can't be solved by the Boussinesq approximation, which is commonly used in CFD field. This study adopted a non-Boussinesq modeling to simulate multi-fluid or large temperature-gradient-driven flow more realistically. In this model, the reference density is defined by the particle temperature and particle mass is changed accordingly [6].

Table I. SPH formulated models of SOPHIA code

Mass conservation
$\left(\frac{\rho}{\rho_{ref}}\right)_i = \sum_j \frac{m_j}{\rho_{ref,j}} W_{ij}$ (3)
$\frac{d}{dt}\left(\frac{\rho}{\rho_{ref}}\right)_i = -\left(\frac{\rho_i}{\rho_{ref,i}}\right)\sum_j \frac{m_j}{\rho_j}(\boldsymbol{u}_i - \boldsymbol{u}_j)\cdot\nabla W_{ij}$ (4)
Momentum conservation
$\left(\frac{d\boldsymbol{u}}{dt}\right)_i = \left(\frac{d\boldsymbol{u}}{dt}\right)_i^{fp} + \left(\frac{d\boldsymbol{u}}{dt}\right)_i^{fv} + \boldsymbol{g} + \boldsymbol{f}_{ext}$ (5)
$\left(\frac{d\boldsymbol{u}}{dt}\right)_i^{fp} = -\sum_j m_j \left(\frac{p_i + p_j}{\rho_i \rho_j}\right)\nabla W_{ij}$ (6)
$\left(\frac{d\boldsymbol{u}}{dt}\right)_i^{fv} = \sum_j \frac{4m_j}{\rho_i \rho_j}\left(\frac{\mu_i \mu_j}{\mu_i + \mu_j}\right)(\boldsymbol{u}_i - \boldsymbol{u}_j)\frac{\boldsymbol{r}_{ij}}{\lvert\boldsymbol{r}_{ij}\rvert^2}\cdot\nabla W_{ij}$ (7)
Energy conservation
$\left(\frac{dh}{dt}\right)_i = \sum_j \frac{4m_j}{\rho_i \rho_j}\left(\frac{k_i k}{k_i + k_j}\right)(T_i - T_j)\frac{\boldsymbol{r}_{ij}}{\lvert\boldsymbol{r}_{ij}\rvert^2}\cdot\nabla W_{ij} + \dot{q}_t$ (8)
Equation of State
$p_i = \frac{{c_0}^2 \rho_{ref,i}}{\gamma}\left[\left(\frac{\rho_i}{\rho_{ref,i}}\right)^{\gamma} - 1\right]$ (9)

*$\rho_{ref}, u, g, f_{ext}, p, \mu, h, k,$ and T denote the reference density, velocity vector, gravitational acceleration, external body force, pressure, dynamic viscosity, specific enthalpy, conductivity, and temperature, respectively.

$$\rho_{ref,i} = \rho_{o,i}\left(1 - \alpha_T(T_i - T_{ref,i})\right) \quad (10)$$

$$m_i = \rho_{ref,i} \cdot V_{0,i} \quad (11)$$

where $\rho_0, \alpha_T, T_{ref}$ and V_0 denote the initial density, thermal expansion coefficient, reference temperature, and particle volume. This reference density is applied into the density equations (Eq. (3),(4)), and hence the density change is directly estimated. Finally, as the changed density is incorporated into the governing equations, this approach represents the real physics more accurately beyond the Boussinesq approximation [6].

2.3.3 MARS Coupling implementation

Figure 3 shows the modified algorithm of SOPHIA code for MARS coupling. Data transfer with MARS code is carried out at the end of the loop, in the order of (1) heat flux calculation and data sending, and (2) data receiving and interpolation of wall temperature. First, after time integration, the heat flux of inner wall is calculated using the value of the next time step. For each MARS node, the enthalpy time variation of wall particles are summed and divided by wall area as follows.

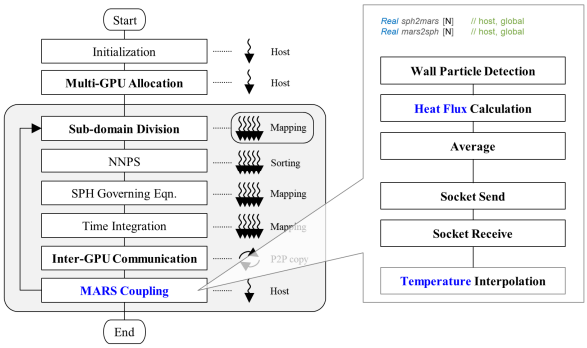


Fig. 3. Modified SOPHIA algorithm for MARS coupling.

$$q'_{m\ ars,k} = \left(\sum_{N_k} \frac{dH_i}{dt}\right) \times \frac{1}{A_k} \quad (12)$$

where $q'_{m\ ars}$, H, and A denote the heat flux value for MARS node, the enthalpy time variation of wall particle, and the inner wall surface area, respectively. The subscript k indicates the index of MARS node and N_k represents the number of SPH particles located in that MARS code.

Next, the temperature distribution received from the MARS is linearly interpolated with the height of wall particles according to the angle of the node. The calculated temperature is given as the constant boundary condition of the next time step.

2.4 Preliminary Simulation Model

This study simulated the hypothetical IVR-ERVC accident in the APR 1400 reactor design. The inner diameter of the reactor vessel is 4.74m and the height is 2.37m. The vessel has combined shape of the spherical with a height of 2m and the cylindrical. This vessel is filled with the corium of oxide-metal mixture corium. The configuration of the corium was referred to ERP input, but the parameters/properties are scaled/adjusted. These two fluids are initially stratified, the upper part for metal with the height of 0.38m and the lower part for oxide with the height of 1.91m. Table 2 show the physical properties of the corium and the input conditions for the preliminary simulation. The upper surface of a metal corium is open as free surface considering radiative heat transfer. For simulating crust formation, the phase change of melt corium to crust is modeled by drastically increasing the viscosity of the particles whose temperature is below the liquidus temperature, which is adjusted as a proper temperature provisionally.

3. Results

Figure 4 shows the simulation results of the in-vessel retention of the oxide-metal corium mixture. The color black presents the molten metal core and color gray presents the molten oxide core. As shown in figure, the decay heat of oxide core heats up the entire fluid rapidly.

Table II. Simulation model and conditions

Parameter		Value
Molten Ceramic Core	Density (kg/m^3)	8191
	Viscosity (Pa·s)	20.48
	Thermal exp. coefficient	1.0×10^{-3}
	Conductivity (W/m·K)	15.0
	Thermal diffusivity (m^2/s)	0.003
	Specific heat (J/kg·K)	0.5
Molten Metal Core	Density (kg/m^3)	2000
	Viscosity (Pa·s)	200.0
	Thermal exp. coefficient	1.0×10^{-3}
	Conductivity (W/m·K)	30.0
	Thermal diffusivity (m^2/s)	0.03
	Specific heat (J/kg·K)	0.5
Volumetric heating power (W/m^3)		1.3×10^{4}
Rayleigh number (Ra)		5.21×10^{5}
Prandtl number (Pr)		0.68

During the accident, the thermal load is transferred from the oxide core to the metal core, and it is removed by external cooling. Due to the high heating power, the temperature of the oxide and metal corium increases, and the density of both fluids decreased because of the thermal expansion. This density gradient field causes the convective flow; the metal core with the relatively high density descends along the inner wall surface, and the oxide core with the relatively low density rises up at the center of the vessel. As a result, the corium pool is evaluated to have a maximum temperature of about 1500K with a high velocity at the wall and center. In addition, as shown in figure, the vigorous mixing occurs at the interface of the two fluids. This is because the density becomes overturned due to the large temperature gradient at the interfaces. That is, it is confirmed that the Lagrangian-based simulation enables to clearly resolve the complicated interfacial motion of multi-fluid having different densities.

4. Conclusions

This study developed an integrated code that couples SOPHIA code (Lagrangian particle-based CFD code) with MARS code (Nuclear reactor system code) in order to simulate the IVR-ERVC phenomena more realistically and provide the best estimate of the safety analysis. The SOPHIA code analyzes the in-vessel corium behavior which involved various complicated phenomena such as natural convection, heat transfer, stratification/mixing of the mixture corium, etc. The MARS code analyzes the external vessel cooling system and two-phase natural circulation flow. These two codes are connected through the socket network and they exchange the data each other. By coupling the two codes, this study enables to handle the real-scale IVR-ERVC accident effectively and efficiently. Using the developed code, the preliminary simulation referring the ERP input was carried out and the results show the reasonable thermal-hydraulic flow motion of the in-vessel corium. Therefore, SOPHIA-

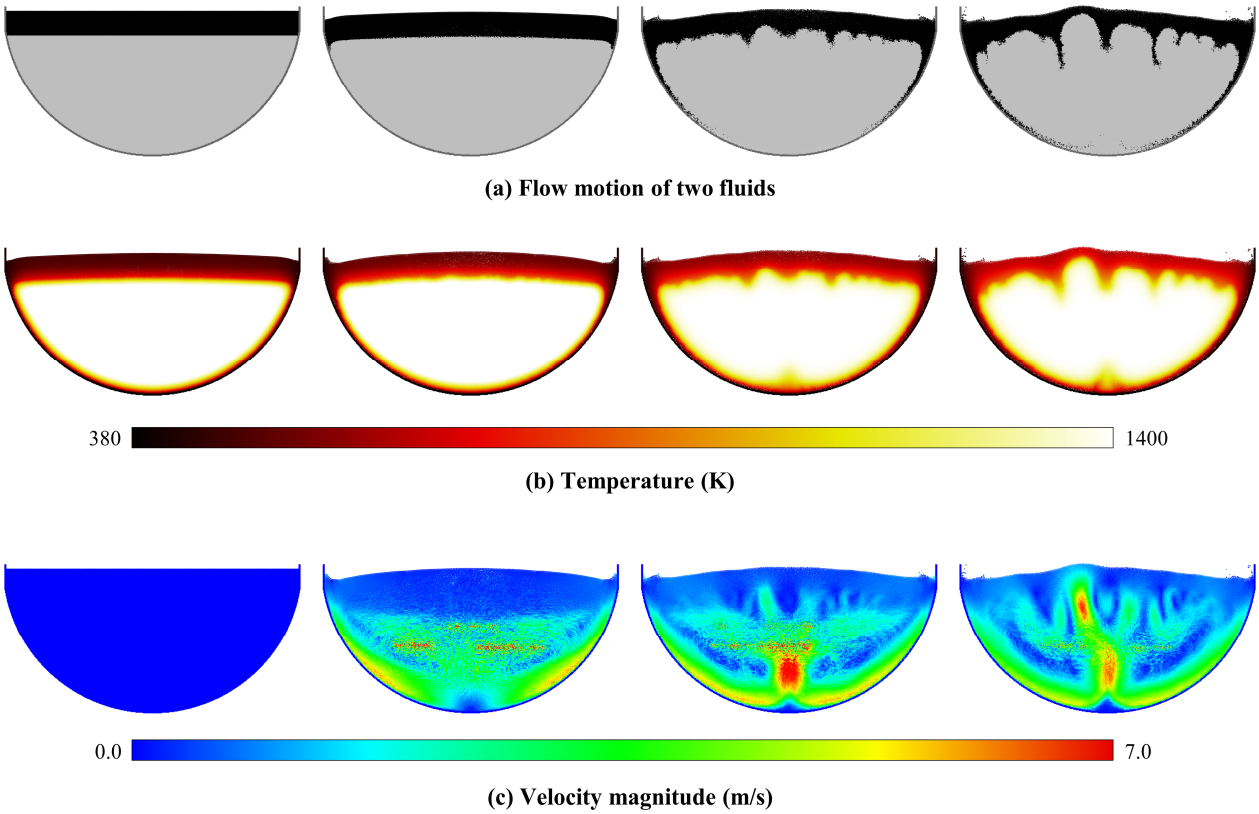


Fig. 4. Snapshots of the preliminary simulation on the IVR-ERVC with the oxide and metal corium mixture: (a) flow motion of corium mixture, (b) temperature distribution, (c) velocity distribution.

MARS integrated code is expected to evaluate the IVR-ERVC phenomena accurately and provide highly reliable visualizations that were rarely observed by conventional CFD method. For the future work, the real-scale oxide/metal corium properties will be adopted and the analysis on the In-vessel Retention will be performed under the proper hypothetical severe accident scenario of APR 1400.

ACKNOWLEDGEMENT

This research was supported by the Nuclear Safety Research Program through the Korea Foundation Of Nuclear Safety (KoFONS) using the financial resource granted by the Nuclear Safety and Security Commission(NSSC) of the Republic of Korea. (No. 1903003)

REFERENCES

[1] Ma, W., Yuan, Y., & Sehgal, B. R. (2016). In-vessel melt retention of pressurized water reactors: historical review and future research needs. *Engineering,* 2(1), 103-111.
[2] Park, R. J., Ha, K. S., & Kim, H. Y. (2016). Detailed evaluation of natural circulation mass flow rate in the annular gap between the outer reactor vessel wall and insulation under IVR-ERVC. *Annals of Nuclear Energy,* 89, 50-55.
[3] Monaghan, J. J. (2005). Smoothed particle hydrodynamics. *Reports on progress in physics*, 68(8), 1703.
[4] Jo, Y. B., Park, S. H., Choi, H. Y., Jung, H. W., Kim, Y. J., & Kim, E. S. (2019). SOPHIA: Development of Lagrangian-based CFD code for nuclear thermal-hydraulics and safety applications. *Annals of Nuclear Energy*, 124, 132-149.
[5] Dehnen, W., & Aly, H. (2012). Improving convergence in smoothed particle hydrodynamics simulations without pairing instability. *Monthly Notices of the Royal Astronomical Society*, 425(2), 1068-1082.
[6] Park, S.H., Chae, H., Jo, Y. B., and Kim, Y. S. (2019). SPH for general density gradient driven flow. *In Proceedings of the 14th SPHERIC International Workshop*, Exeter, United Kingdom, 2019, 67-75.
[7] Park, S.H., Jo, Y. B., and Kim, Y. S. (2019). Development of multi-GPU based smoothed particle hydrodynamics code (SOPHIA Plus) for high-resolution and large-scale simulation on nuclear safety-related phenomena. *In Proceedings of the Korean Nuclear Society Spring Meeting*, Jeju, Republic of Korea, 2019.