

Numerical Simulation of Natural Circulation in a Closed-Loop System Using the Moving Particle Semi-implicit Method

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1. Introduction

Passive safety systems have received increasing attention because they can remove decay heat using natural forces, such as gravity and natural circulation, without external power. Representative reactor concepts under development in Korea include the innovative Small Modular Reactor (i-SMR) and the Passive Molten Salt Fast Reactor (PMFR). The i-SMR adopts passive cooling systems based on natural circulation, while the PMFR uses natural circulation of molten fuel salt as its primary heat transport mechanism and considers passive air cooling for decay heat removal [1,2].

In molten salt reactors, phase change such as solidification of molten salt can occur during cooling conditions. The formation and movement of the solid-liquid interface can affect heat transfer and flow behavior. Therefore, a numerical method capable of handling evolving phase interfaces is required for the analysis of molten salt systems involving phase change.

The Moving Particle Semi-implicit (MPS) method is a mesh-free Lagrangian particle method originally developed for incompressible flows with free surfaces and large deformation [3]. Unlike conventional grid-based methods, the MPS method represents the computational domain using particles, allowing moving interfaces to be treated without mesh deformation. Therefore, the MPS method can be extended to the analysis of phase-change phenomena in molten salt systems.

In this study, natural circulation in a simplified single-phase closed loop without a free surface is simulated using the MPS method. The present analysis evaluates the applicability of the MPS method to buoyancy-driven flow and heat transfer in a closed domain as a preliminary step toward phase-change analysis of molten salt systems.

2. Numerical Methodology

2.1 Governing Equations and MPS Formulation

The working fluid was assumed to be a single-phase incompressible Newtonian fluid. The thermophysical properties were treated as constant, except for the density variation associated with the buoyancy force. The

governing equations in the Lagrangian framework are expressed as

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

$$\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho_0} \nabla p + \nu \nabla^2 \mathbf{u} - \beta(T - T_{\text{ref}}) \mathbf{g}, \quad (2)$$

and

$$\frac{DT}{Dt} = \alpha \nabla^2 T, \quad (3)$$

where $\mathbf{u}$ is velocity; p is pressure; T is temperature; ρ_0 is the reference density; ν is kinematic viscosity; α is thermal diffusivity; β is volumetric thermal expansion coefficient; $\mathbf{g}$ is the gravitational acceleration vector; T_{ref} is the reference temperature. The Boussinesq approximation was employed, with the density variations considered only in the buoyancy term. The reference hydrostatic pressure was incorporated into p . Heating and cooling were imposed through the thermal boundary conditions described in Section 2.3.

In the MPS method, the governing equations are discretized through interactions between neighboring particles [3]. The interaction strength between particles i and j is determined using the weight function

$$w(r_{ij}) = \begin{cases} \frac{r_e}{r_{ij}} - 1, & 0 < r_{ij} < r_e, \\ 0, & r_{ij} \geq r_e, \end{cases} \quad (4)$$

where $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$ is the distance between the particles and r_e is the effective interaction radius. The particle number density is calculated as

$$n_i = \sum_{j \neq i} w(r_{ij}), \quad (5)$$

and its reference value n^0 , obtained from the initial uniform particle arrangement, is used to impose incompressibility.

The pressure-gradient and Laplacian operators are discretized as [3]

$$\langle \nabla p \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \frac{p_j - p_i}{r_{ij}^2} (\mathbf{r}_j - \mathbf{r}_i) w(r_{ij}), \quad (6)$$

$$\langle \nabla^2 \phi \rangle_i = \frac{2d}{\lambda n^0} \sum_{j \neq i} (\phi_j - \phi_i) w(r_{ij}), \quad (7)$$

where d is the number of spatial dimensions, ϕ represents velocity or temperature, and λ is a

normalization parameter defined from the initial particle arrangement as

$$\lambda = \frac{\sum_{j \neq i} r_{ij}^2 w(r_{ij})}{\sum_{j \neq i} w(r_{ij})}. \quad (8)$$

A semi-implicit prediction-correction procedure was used for the fluid calculation. In the prediction step, the viscous and buoyancy terms were evaluated explicitly to obtain the intermediate velocity and particle positions. The pressure at the next time step was then obtained from the pressure Poisson equation

$$\langle \nabla^2 p^{n+1} \rangle_i = -\frac{\rho_0(n_i^* - n^0)}{\Delta t^2 n^0}, \quad (9)$$

where n_i^* is the particle number density calculated using the predicted particle positions. The velocity was subsequently corrected as

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^* - \frac{\Delta t}{\rho_0} \langle \nabla p^{n+1} \rangle_i. \quad (10)$$

The temperature field was calculated using the same MPS Laplacian model used for the viscous term. Because the particles move with the fluid velocity, the advection terms do not require separate spatial discretization. The resulting temperature-dependent buoyancy force drives the natural-circulation flow through the closed loop.

2.2 Natural Circulation Loop Model

The computational domain was a two-dimensional rectangular closed loop adapted from the natural-circulation mini-loop geometry reported by Misale et al. [4]. The reference was used only as the geometric basis of the present model; its experimental results were not used for comparison. The reported centerline-length-to-diameter ratio of 165.5 and height-to-width ratio of 0.87 were adopted as the defining geometric parameters. With a channel gap of 4 mm and a bend centerline radius of 22 mm, the horizontal and vertical straight lengths were determined to be 143.1 and 118.8 mm, respectively. The resulting loop had an overall width of 187.1 mm, a height of 162.8 mm, and a centerline length of 662 mm. The 139 mm heat-transfer sections were centered in the upper and lower horizontal legs (Table I). The resulting loop geometry and the locations of the heating and cooling sections are shown in Fig. 1.

The loop was filled with single-phase water and modeled without the expansion tank and free surface of the reference facility. Heating and cooling were represented by prescribed-temperature wall particles, as described in Section 2.3. Accordingly, the present model constitutes a simplified two-dimensional closed-loop system rather than a numerical reproduction of the experiment.

2.3 Initial and Boundary Conditions

Initially, the fluid and tube-wall particles were uniformly set to 25 °C, and the fluid was at rest. The initial pressure field was specified using a hydrostatic

distribution, with the gauge pressure at the uppermost fluid location set to 0 Pa. Gravity was applied in the vertically downward direction.

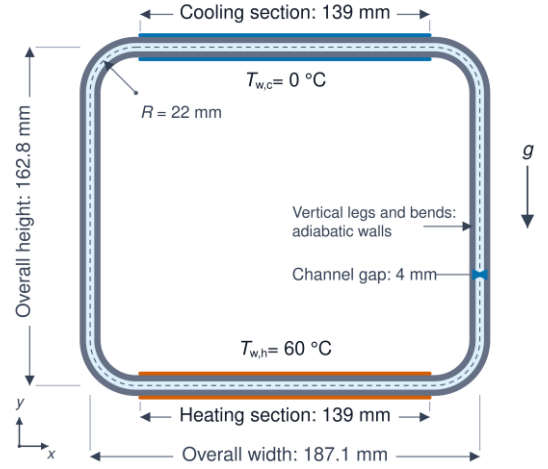


Fig. 1. Geometry and thermal boundary conditions of the two-dimensional natural circulation loop.

Table I: Geometric parameters of the two-dimensional natural circulation loop.

Parameter	Value	Basis
Centerline length-to-diameter ratio, L/D	165.5	Ref. [4]
Height-to-width ratio, H/W	0.87	Ref. [4]
Channel gap, w	4 mm	Ref. [4]
Heating / cooling section length, $L_h = L_c$	139 mm	Ref. [4]
Bend centerline radius, R	22 mm	Assumed
Overall width, W	187.1 mm	Derived
Overall height, H	162.8 mm	Derived
Loop centerline length, L	662 mm	Derived
Hydraulic diameter, $D_h = 2w$	8 mm	Derived

Table II: Initial and boundary conditions of the loop model.

Item	Specification
Initial condition ($t = 0$)	
Temperature	25 °C
Velocity	At rest (0 m/s)
Pressure	0 Pa gauge at the uppermost fluid location
Thermal boundary condition ($t > 0$)	
Heater wall	$T_{w,h} = 60$ °C
Cooler wall	$T_{w,c} = 0$ °C
Other walls	Adiabatic

At $t = 0$, the temperatures of the heating- and cooling-wall particles were fixed at 60 and 0 °C, respectively, and maintained constant throughout the calculation. Heat transfer between the fluid and adjacent wall particles was calculated by thermal conduction. The vertical sections

and bends, excluding the heating and cooling sections, were treated as adiabatic boundaries; thus, no heat transfer to the exterior of the loop was allowed in these regions.

A no-slip condition was imposed on all tube walls. The tube walls were represented by two layers of wall particles, and no dummy particles were used. Additional layers of constant-temperature wall particles were placed outside the upper and lower tube walls in both the heating and cooling sections.

The buoyancy force was evaluated using the Boussinesq approximation with a reference temperature of 25 °C (298.15 K). The thermal expansion coefficient, β , was prescribed as a piecewise-linear function of temperature. Because the loop geometry and thermal boundary conditions were symmetric, no preferential circulation direction was imposed, allowing either clockwise or counter-clockwise circulation to develop. (Table II)

2.4 Numerical Conditions and Verification Criteria

The two-dimensional loop was discretized using a nominal particle spacing of $l_0 = 0.5$ mm. The effective interaction radii were set to $3.1l_0$ for the particle number density and pressure gradient, and $4.0l_0$ for the Laplacian operators. The fluid was represented by 11,500 water particles.

The pressure Poisson equation was solved using the conjugate-gradient method. The time step was adjusted according to Courant and diffusion numbers of 0.05 and 0.2, respectively, with a maximum time step of 2.0×10^{-4} s. The transient calculation was conducted up to 300 s.

The buoyancy-induced density variation of water was evaluated using a piecewise-linear volumetric thermal-expansion model over 0-60 °C, with a reference temperature of 25 °C. Because the transport properties were held constant, the dynamic viscosity and thermal conductivity were evaluated at the loop-mean fluid temperature obtained from the calculation itself, 32.6 °C, giving a Prandtl number of 5.16. The reference density in Table III corresponds to the buoyancy reference temperature of 25 °C.

Table III: Thermophysical properties used in the calculation.

Material	ρ (kg/m ³)	μ (Pa · s)	k (W/m · K)	c_p (J/kg · K)
Water	996.5	0.765×10^{-3}	0.62	4,186
Copper	8,960	N/A	401	385

The loop-averaged speed was defined as the magnitude of the particle-number-averaged tangential velocity over the four straight legs. The flux-consistent bulk velocity was calculated from the mean of the four leg fluxes multiplied by the loop centerline length of 0.662 m and divided by the number of water particles, 11,500.

Quasi-steady conditions were identified by requiring the loop-averaged speed and the leg temperatures to remain within 1% of their window means. Verification is based on two independent checks: symmetry of the riser and downcomer mass flow rates, and comparison of the flux-consistent bulk velocity with a reduced-order one-dimensional buoyancy-friction balance.

3. Results and Verification

3.1 Development of Natural Circulation

Fig. 2 shows the transient response of the natural-circulation loop following the application of the prescribed wall temperatures. The loop-averaged speed remained low during the initial thermal-development period. After approximately 40 s, the growing temperature difference between the two vertical legs produced a significant buoyancy driving force, and the loop-averaged speed reached approximately 36.4 mm/s at about 50 s. This initial peak was followed by an undershoot to 12.8 mm/s at 61 s and damped oscillations.

The loop-averaged speed and leg temperatures exhibited coupled oscillations. As these oscillations decayed, the right and left legs became the hot riser and cold downcomer, respectively. After approximately 120 s, the loop approached a quasi-steady condition. The loop-averaged speed was 22.0 mm/s, while the mean riser and downcomer temperatures were 43.3 and 22.0 °C, respectively, giving a temperature difference of approximately 21 °C. These results confirm that stable buoyancy-driven circulation was established in the closed loop.

3.2 Steady-State Flow and Temperature Distribution

The steady-state fields were evaluated over 200-300 s. The loop-averaged speed was 22.02 ± 0.18 mm/s, and the mean riser and downcomer temperatures were 43.26 ± 0.05 and 22.03 ± 0.04 °C, respectively. These small temporal variations confirm that the selected interval represents a quasi-steady state.

As shown in Fig. 3, the fluid temperature increased from 26.2 °C at the heated-section inlet to 43.7 °C at its outlet, corresponding to a temperature rise of 17.5 °C. The hot fluid subsequently ascended through the riser, whose bulk mean temperature was 43.3 °C. In the cooled section, the temperature decreased from 38.9 to 20.7 °C, while the downcomer bulk temperature was 22.0 °C. The temperature changes in the two bends before the prescribed-temperature sections suggest the influence of axial heat conduction through the copper wall.

3.3 Steady-State Flow Verification

The mean mass flow rates through the riser and downcomer were +0.0938 and -0.0960 kg/s, respectively, giving a 2.38% difference in magnitude. The flux-consistent bulk velocity was 22.0 mm/s. Using the 8 mm

hydraulic diameter of the two-dimensional parallel-plate channel gives $Re = 229$, confirming laminar circulation.

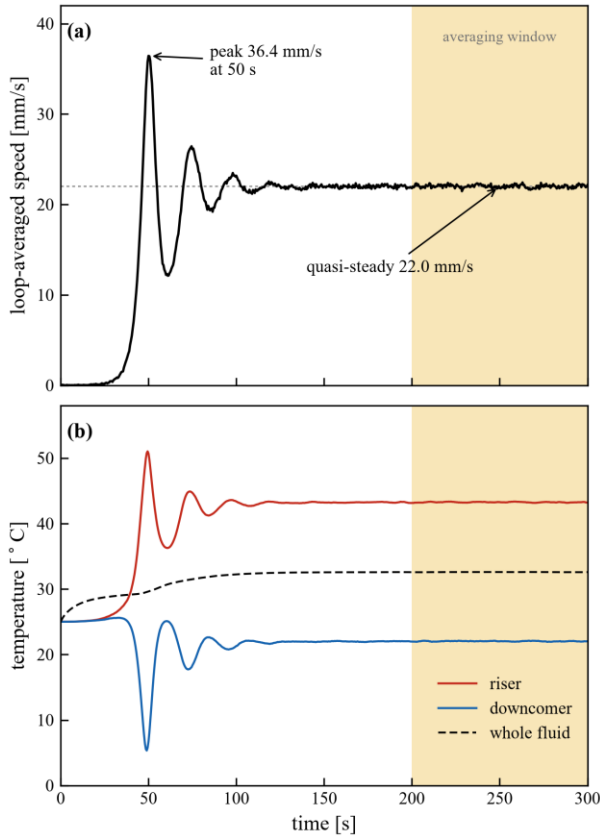


Fig. 2. Transient histories of (a) the loop-averaged speed and (b) mean loop and two leg temperatures.

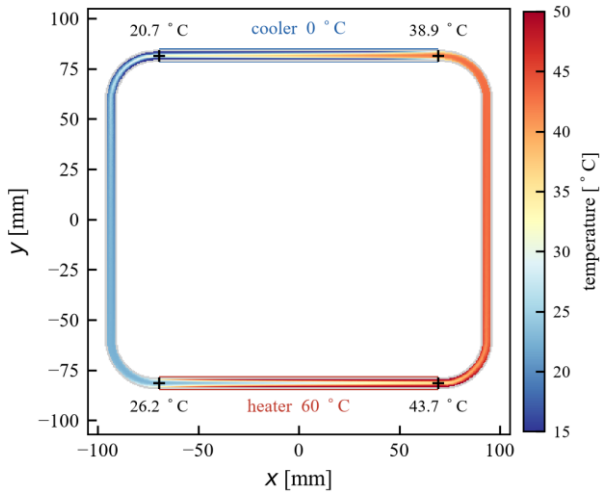


Fig. 3. Time-averaged fluid-temperature field over 200-300 s.

For a reduced-order momentum check, the density model gave mean riser and downcomer densities of 990.4 and 997.2 kg/m^3 . The corresponding buoyancy head over the 0.1628 m vertical height was 10.85 Pa, whereas the fully developed parallel-plate friction loss over the 0.662 m loop was 8.36 Pa at the MPS bulk velocity. When bend/form losses are neglected, the one-dimensional balance predicts 28.56 mm/s, and the MPS

flux-consistent bulk velocity of 22.0 mm/s is 22.9% lower than that prediction.

To obtain a geometry-specific bend loss, additional isothermal forced-flow MPS simulations of a two-bend duct and a matched straight duct were compared at the same centerline locations. The pointwise difference isolated the bend loss without assuming a friction correlation. At $Re \approx 256$, the simulations gave $f \cdot Re = 89.2$ and $K_{local} = 1.21$ per bend.

At quasi-steady state, the buoyancy head is balanced by the distributed friction and local form losses [5]. Using $f = 89.2/Re$, $Re = \rho U D_h / \mu$, and $K_\Sigma = 4K_{local} = 4.84$, the one-dimensional momentum balance becomes:

$$\Delta P_b = \frac{44.6\mu L}{D_h^2} U + K_\Sigma \frac{\rho U^2}{2}. \quad (11)$$

Solving Eq. (11) with the present fluid properties and loop dimensions yields a one-dimensional bulk velocity of 26.1 mm/s. The MPS flux-consistent bulk velocity of 22.0 mm/s is 15.7% lower than this prediction, compared with 22.9% when bend losses are omitted. Thus, the independently evaluated bend losses reduce the difference.

Because K_{local} was evaluated at a single Reynolds number using an isothermal auxiliary simulation, it is treated here as a code-consistent verification parameter rather than an experimentally validated coefficient. The remaining difference may reflect developing and multidimensional flow effects and spatially varying fluid properties that are not represented in the one-dimensional balance.

4. Conclusions

The MPS method was applied to a two-dimensional, single-phase closed loop to evaluate its capability for simulating buoyancy-driven natural circulation. The calculation simulated transient development and quasi-steady circulation behavior, with consistent mass flow rates through the riser and downcomer. Comparison with a reduced-order one-dimensional momentum balance showed that the MPS flux-consistent bulk velocity was 15.7% lower than the one-dimensional prediction. This result may reflect multidimensional flow effects in the loop geometry that are not represented in the reduced-order model.

The present results demonstrate the applicability of the MPS method to closed-loop natural circulation and provide a basis for its extension to molten salt systems involving phase-change phenomena. However, the present analysis is limited by the two-dimensional single-phase model, simplified boundary conditions, and the absence of particle-spacing and time-step sensitivity studies. Future work will include comparison with experimental natural-circulation data and extension of the MPS model to phase-change conditions relevant to molten salt systems.

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