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# Numerical study on a heat transfer model in a Lagrangian fluid dynamics simulation

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ABSTRACT

Phenomena related to phase change heat transfer are often encountered in engineering. These phenomena are regarded to be complex, since not only phase transition from solid to liquid occurs but also movement of fluid interface has to be taken into consideration. Detailed numerical modeling of these complex systems is essential to better understand them and optimize industrial designs. Lagrangian methods are promising for simulating such complex systems. The Moving Particle Semi-implicit (MPS) method, which is one of the Lagrangian methods, is employed here to simulate the free surface fluid flows involving heat transfer and phase change. On the other hand, the existing MPS method could not apply Neumann boundary condition such as heat flux in the heat transfer simulations. This is because the surface direction could not be readily defined on the surface of the spherical fluid particles in the MPS method. Hence, prescribing the heat fluxes becomes problematic in the existing MPS method. To solve this problem, a new heat flux model is developed, where the divergence operator is applied in the heat transfer simulation. Simple verification tests are performed to demonstrate the heat flux model, where the calculation results are compared against analytically derived solutions. In addition, application of the signed distance function is also investigated in the heat transfer simulation for arbitrary shaped boundary. In simple verification tests, the computation results are shown to agree well with the analytical solutions. Consequently, adequacy of the novel heat transfer model developed here is shown in the Lagrangian fluid dynamics simulation.



## 1. Introduction

Phase change heat transfer is often encountered in various engineering [1–3] such as chemical engineering, food engineering, mechanical engineering, nuclear engineering, resilience engineering, etc. At present, introduction of numerical technologies are desired for accurate product design and/or better understanding of the phenomena. When phase change heat transfer phenomena are numerically simulated, not only heat transfer model but also interfacial fluid flow modeling is required. For modeling the interfacial fluid flow, the Volume-of-Fluid (VOF) [4–8], Smoothed Particle Hydrodynamics (SPH) [9–12] and Moving Particle Semi-implicit (MPS) method [13–15] have been employed in the computations so far. Lagrangian methods such as the SPH and MPS method are regarded to be accurate in simulating free surface fluid flows, since convection term is not required in the modeling. Accordingly, the Lagrangian approach becomes important in various engineering. Recently, weakly compressible MPS method [16,17] was developed for efficient calculation of the interfacial flows, where the pressure computation was performed explicitly. Hence, the calculation efficiency of the MPS method has been improved substantially and is now capable of industrial application. The MPS method was applied to complex thermal hydraulic systems such as a simulation of a severe accident in nuclear engineering [18,19]. Although the MPS method seems to be established, there are some issues in the heat transfer simulations. Specifically, in the existing MPS method, Neumann boundary condition such as heat flux boundary could not be set. This is because the surface direction could not be evaluated easily at the surface of MPS particles, and hence heat flux could not be set at the boundary. Only Dirichlet boundary could be used in the existing MPS method [18–21], and thus only the temperature could be set at the boundary. In addition, in the existing MPS method, accuracy

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**Nomenclature**

| | |
|---|---|
| $C$ | empirical constant for viscosity [–] |
| $c$ | sound speed [m/s] |
| $c_p$ | specific heat [J/(kg K)] |
| $D$ | dimension number [–] |
| $\boldsymbol{g}$ | gravitational acceleration [m/s$^2$] |
| $h$ | enthalpy [J/m$^3$] |
| $k$ | thermal conductivity [W/(m K)] |
| $L$ | latent heat [J/kg] |
| $l$ | length [m] |
| $\boldsymbol{N}$ | unit void vector [–] |
| $n$ | particle number density [–] |
| $n^0$ | initial particle number density [–] |
| $P$ | pressure [N/m$^2$] |
| $Q$ | heat source [J/m$^3$] |
| $q$ | heat flux vector [W/m$^2$] |
| $\boldsymbol{r}$ | coordinate vector [m] |
| $r$ | distance [m] |
| $r_e$ | cutoff radius [m] |
| $T$ | temperature [K] |
| $T_m$ | melting point [K] |
| $t$ | time [s] |
| $\boldsymbol{u}$ | fluid velocity [m/s] |
| $w$ | basic kernel function [–] |
| $w_g$ | special kernel function for pressure gradient [–] |

*Greek symbols*

| | |
|---|---|
| $\Phi$ | variable [–] |
| $\gamma$ | phase fraction [–] |
| $\Gamma$ | constant for surface detection [–] |
| $\lambda$ | Laplacian constant in the MPS method [–] |
| $\mu$ | viscosity [Pa s] |
| $\nu$ | fluid kinematic viscosity [m$^2$/s] |
| $\tau$ | viscous tensor |
| $\rho$ | fluid density [kg/m$^3$] |

*Subscript*

| | |
|---|---|
| $i, j$ | particle number |
| $L$ | liquid phase |
| $S$ | solid phase |
| *Wall* | property of wall |
| *Max* | maximum property |
| 1,2 | type number |

*Superscript*

| | |
|---|---|
| $*$ | auxiliary value |

of the heat transfer calculation is known to be worse in arbitrary shape wall systems. This is because the wall boundary was created by stepwise location of the MPS particles. Consequently, the existing MPS method has problems in heat transfer simulation.

To solve the above issues, novel heat transfer model is developed in the MPS method. Specifically, heat flux model is newly developed in the current study. The weakly compressive MPS method is used in this study. To apply the MPS simulation of heat transfer in an arbitrary shaped domain, the signed distance function (SDF) is introduced for the first time. In addition, the implicit calculation algorithm [22] is newly introduced into the MPS method to simulate highly viscous fluid flow involving heat transfer efficiently. Verification tests are performed in a simple system to prove adequacy of the new models. Calculation results agree well with theoretical ones. Moreover, the numerical model is shown to simulate phase change system. Thus, the new heat transfer model is verified in Lagrangian fluid dynamics.

## 2. Methodology

### 2.1. The governing equations

For the weakly compressible fluid motion, the mass and momentum conservation equations can be written as

$$\frac{D\rho}{Dt} + \rho\nabla\cdot\boldsymbol{u} = 0, \tag{1}$$

$$\frac{D\boldsymbol{u}}{Dt} = -\frac{1}{\rho}\nabla P + \nabla\cdot\boldsymbol{\tau} + \boldsymbol{g}, \tag{2}$$

where $\rho$, $t$, $\boldsymbol{u}$, $P$, $\boldsymbol{\tau}$ and $\boldsymbol{g}$ are the fluid density, time, fluid velocity, pressure, viscous tensor and gravity, respectively. The $\boldsymbol{\tau}$ is given by $\boldsymbol{\tau} = \nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T$.

Considering heat transfer, the energy conservation equation is given as follows:

$$\frac{Dh}{Dt} = \nabla\cdot(k\nabla T) + Q, \tag{3}$$

where $h$, $k$, $T$ and $Q$ are the enthalpy, thermal conductivity, temperature and energy inflow, respectively.

### 2.2. The MPS method

In the MPS method [13], the differential operator is modeled by the weighted average between neighbor particles. A basic kernel function is given [16,17] as

$$w(r) = \begin{cases} \frac{r}{r_e} + \frac{r_e}{r} - 2 & r < r_e \\ 0 & r \geqslant r_e \end{cases}, \tag{4}$$

where $r$ and $r_e$ are distance and cutoff radius of interaction, respectively. Assuming that virtual particles are set in a structurally aligned particle gird, the initial particle number density and Laplacian constant are given as

$$n^0 = \sum_{j\neq i} w(|\boldsymbol{r}_j - \boldsymbol{r}_i|), \tag{5}$$

$$\lambda = \frac{1}{n^0}\sum_{j\neq i} |\boldsymbol{r}_j - \boldsymbol{r}_i|^2 w(|\boldsymbol{r}_j - \boldsymbol{r}_i|). \tag{6}$$

These values are constant during the calculation. The particle density can be approximated to be proportional to the initial particle number density as follows:

$$n_i = \sum_{j\neq i} w(|\boldsymbol{r}_j - \boldsymbol{r}_i|), \tag{7}$$

$$\rho_i = \frac{n_i}{n^0}\rho_0. \tag{8}$$

In the weakly compressible approach [16,17], pressure can be derived as a function of density and is given by