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Stable mesh-free moving particle semi-implicit method for direct analysis of gas–liquid two-phase flow

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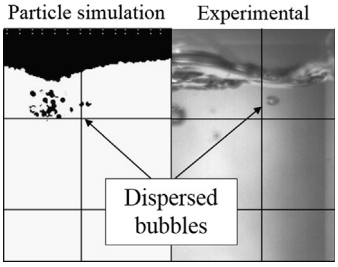
HIGHLIGHTS

- Mesh-free particle simulation was performed for Direct Analysis of gas–liquid two-phase flow and dispersion behavior.
- The gas–liquid interface was simulated with high accuracy and volume conservation.
- This simulation model was verified by comparison with a cold model experiment on the same scale.
- The stability of the interface was improved by introducing weak compressibility and a smooth density function.
- Higher filling ratio arrangement could maintain the standard particle number density as the condition of an incompressible fluid.

GRAPHICAL ABSTRACT



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ABSTRACT

In a metallurgical process, gas–liquid flow plays an important role in increasing the efficiency by stirring liquid mechanically or by injecting a gas. Owing to the difficulty of direct observation in a high-temperature system or real furnace experiment, numerical analysis is useful and widely studied. However, flexible treatment of complicated free surface behavior such as fragmentation and coalescence of liquids is still a difficult problem. This paper presents a new particle-based simulation scheme for gas–liquid flow. We improved the numerical stability, which is generally a problem with the particle method, and verified the model's accuracy for fundamental gas–liquid flow analysis.

Because all the phases were discretized as particles in Moving Particle Semi-implicit (MPS) method, the proposed model can track the movement of both the gas and liquid phases directly. A large difference in the real density between the gas and liquid phases makes the gas–liquid interface behavior unstable. This study proposed an optimization of the weakly compressible Poisson equation, an initial particle arrangement, and a smoothed interface density in order to stabilize the multi-density flow analysis. This model guarantees conservation of the fluid volume even for a high-density-ratio flow like that at a gas–liquid interface. Therefore, a gas–liquid interface has been represented with high accuracy. We believe that this scheme is also applicable to phenomena in an actual process that includes many dispersal phases.

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1. Introduction

Control of bubbly flow in high-temperature melts is necessary in several material processes. In the steel making or copper smelting processes, the gas flow that passes between the melting metal and the slag affects the reaction rate and refinement efficiency because of the change in the gas–liquid interfacial area (Bird et al., 2006; Nakamura et al., 1988; Sano et al., 1976; Pehlke et al., 1974). Metal electrolysis is also often accompanied by gas–liquid two-phase flow such as gas generation around the anode or reduction of gas at the cathode in a molten salt (Otake et al., 2013). The bubbles that appear in this process rise up inside of the liquid phase by fluid movement owing to the density difference. They frequently show complicated behavior consisting of repeated coalescence and breakup. Microscale bubbles often show decreasing volume instead of forming large bubbles or are adsorbed on a solid surface because the surface tension force becomes relatively large. It is still difficult to control an unsteady three-dimensional gas–liquid flow of these complicated bubbles and the reaction behavior.

To analyze bubble behavior in molten metal or slag at high temperature, in situ observation by high-temperature X-ray penetration equipment has been performed (Nakamura et al., 1988; Han and Holappa, 2003). Visualization of bubbles floating in the melt and surface tension measurement are possible by using this method. However, it is difficult to perform X-ray penetration of the inside of molten metal, and because the observation domain is extremely limited, three-dimensional bubble behavior cannot be determined from two-dimensional observations. Because the flow and mass transfer at the gas–liquid interface depend greatly on the physical properties of the melt and are very complicated, it is difficult to predict these phenomena and optimize the operational conditions without observational data.

The latest progress in computational science and technology raises expectations for a high-accuracy numerical simulation to provide a solution to this complicated problem. The authors have performed numerical simulations of gas, solid, or liquid flow in a packed bed process (Natsui et al., 2011, 2012a, 2012b, 2012c, 2013). Using a large-scale numerical simulation, we can obtain the unsteady three-dimensional information that is difficult to observe experimentally.

Although many computational models of a gas–liquid two-phase flow have been proposed, many problems still remain. Because the interface shape changes with time while the physical properties change discontinuously at a gas–liquid interface, it is difficult to analyze them under microscopic dynamic balance conditions. Thus, a macroscopic two-fluid model that does not calculate the gas–liquid interface shape is still in wide practical use. The two-fluid model requires the application of an empirical formula for the momentum exchange between the gas and the liquid to compensate for the absence of the gas–liquid interface shape calculation, and the calculation accuracy will depend greatly on the reliability of the experimental data.

On the other hand, the interface tracking method is available as an unexperiential approach that can capture the gas–liquid interface form directly. The finite element method (Bonnerot and Jamet, 1977; Lynch, 1982) and a boundary-fitted coordinate system (Ryskin and Leal, 1984a, 1984b) are used to make a calculation cell following interface modification; they require reconstruction of the calculation lattice. The volume of fluid (VOF) method (Hirt and Nichols, 1981), which pursues the share of fluid by the Euler method, is widely known. When the VOF method is applied to a complicated interface and advection of bubbles, a special technique is needed to prevent accumulation of the interface form error by coarse graining, and what is called numerical diffusion. These techniques include the donor–acceptor method (Hirt and Nichols, 1981), level-set method (Osher and Sethian, 1988), CIP method (Takewaki et al., 1985; Yabe and Wang, 1991), PLIC (Rider and Kothe, 1998), MARS method (Kunugi, 1997), and CICSAM (Ubbink and Issa, 1999). These methods each have advantages and disadvantages for reconstruction of the calculation cells, volume conservation, and the interface reconstruction method, so it is necessary to choose the optimal method according to the calculation conditions.

The above-mentioned problems are caused by discretization of cells. The particle method is a Lagrangian approach that does not use a mesh and discretizes the fluid into moving particles; thus, numerical diffusion does not exist in essence. In the particle method, particles themselves move by advection according to their mass and volume. Therefore, the algorithm is simple, and each particle maintains a sharp interface. The smoothed particle hydrodynamics (SPH) method (Lucy, 1977) is a particle method for fluid dynamics. It was originally developed for astrophysical applications and was later expanded for applications in solid and fluid mechanics (Monaghan, 1994). It works by dividing the fluid into a set of discrete elements referred to as particles and is based on integral representation of quantities and spatial derivatives. The SPH method is suitable for a compressive fluid under a noticeable density change. On the other hand, Koshizuka and Oka (1996) proposed the moving particle semi-implicit (MPS) method, which discretized the incompressible Navier–Stokes equation using a Taylor series.

In earlier version of MPS methods, the gas phase movement has been ignored and only the liquid phase has been tracked as a single-phase flow (Koshizuka and Oka, 1996). This avoids the numerical instability caused by a large pressure gradient due to the large density difference. However, new algorithms for solving a multi-density fluid directly have been proposed in recent years. Das and Das (2011) proposed the diffuse interface model for the SPH method to solve a high-density-ratio fluid, and it is also used to explore the physical parameters of such bubbly flows (Das and Das, 2013). Shakibaeinia and Jin (2012) proposed the weakly compressible MPS (WC-MPS) method and applied it to the Rayleigh–Taylor instability problem. They compared it with the VOF method and concluded that the WC-MPS method provides a sharper interface. Although the density ratio of this MPS method was still not large (Khayyer and Gotoh, 2013), their results indicated that this method can be applied to large-scale industrial processes. On the other hand, Colagrossi and Landrini (2003), Grenier et al. (2009; 2013) and Szewc et al. (2013) already applied the multi-phase SPH model to a more practical bubble flow.

In this application of the MPS method, it is necessary to numerically stabilize the gas–liquid interface if it is to be applied to metallurgical processes such as molten metal–slag–gas systems. This paper thus aims to develop a new model based on the multi-phase MPS model for incompressible systems. In this research, the stability of the gas–liquid interface was improved, and we verified the computational accuracy of this model by comparing the numerical results with analytical/experimental results.

2. Numerical and experimental method

2.1. Governing equations of incompressible fluid flow

The governing equations are expressed by the equation of continuity and incompressible Navier–Stokes equation. In the Lagrangian system, they can be written as

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

$$\frac{D\boldsymbol{u}}{Dt}=-\frac{1}{\rho}\nabla p+\nu\nabla^2\boldsymbol{u}+\boldsymbol{g}+\frac{1}{\rho}\boldsymbol{F}_s \tag{2}$$