1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

**Stable Mesh-free Moving Particle Semi-implicit Method
for Direct Analysis of Gas-Liquid Two-Phase Flow**

Shungo Natsui^{*)}, Hifumi Takai, Takehiko Kumagai,
Tatsuya Kikuchi, and Ryosuke O. Suzuki

Division of Materials Science and Engineering,
Faculty of Engineering, Hokkaido University
Kita 13, Nishi 8, Kita-ku, Sapporo, 060-8628 Japan.

*Corresponding author. Tel.: +81-11-706-6342
E-mail address: natsui@eng.hokudai.ac.jp

1 Abstract:

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

14 Because all the phases were discretized as particles in
15 Moving Particle Semi–implicit (MPS) method, the proposed
16 model can track the movement of both the gas and liquid
17 phases directly. A large difference in the real density between
18 the gas and liquid phases makes the gas–liquid interface
19 behavior unstable. This study proposed an optimization of the
20 weakly compressible Poisson equation, an initial particle
21 arrangement, and a smoothed interface density in order to
22 stabilize the multidensity flow analysis. This model guarantees
23 conservation of the fluid volume even for a high–density–ratio

1 flow like that at a gas–liquid interface. Therefore, a gas–liquid
2 interface has been represented with high accuracy. We believe
3 that this scheme is also applicable to phenomena in an actual
4 process that includes many dispersal phases.

5
6 Keywords: Material processing; Moving Particle Semi–
7 implicit method; gas–liquid flow; incompressible flow;
8 dispersion

11 **1. Introduction**

13 Control of bubbly flow in high–temperature melts is
14 necessary in several material processes. In the steel making or
15 copper smelting processes, the gas flow that passes between
16 the melting metal and the slag affects the reaction rate and
17 refinement efficiency because of the change in the gas–liquid
18 interfacial area (Bird et al., 2006; Nakamura et al., 1988; Sano
19 et al., 1976; Pehlke et al., 1974). Metal electrolysis is also often
20 accompanied by gas–liquid two–phase flow such as gas
21 generation around the anode or reduction of gas at the cathode
22 in a molten salt (Otake et al., 2013). The bubbles that appear
23 in this process rise up inside of the liquid phase by fluid

1 movement owing to the density difference. They frequently
2 show complicated behavior consisting of repeated coalescence
3 and breakup. Microscale bubbles often show decreasing
4 volume instead of forming large bubbles or are adsorbed on a
5 solid surface because the surface tension force becomes
6 relatively large. It is still difficult to control an unsteady three-
7 dimensional gas-liquid flow of these complicated bubbles and
8 the reaction behavior.

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

23 The latest progress in computational science and

1 technology raises expectations for a high-accuracy numerical
2 simulation to provide a solution to this complicated problem.
3 The authors have performed numerical simulations of gas,
4 solid, or liquid flow in a packed bed process (Natsui et al., 2011,
5 2012a, 2012b, 2012c, 2013). Using a large-scale numerical
6 simulation, we can obtain the unsteady three-dimensional
7 information that is difficult to observe experimentally.

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

21 On the other hand, the interface tracking method is
22 available as an unexperiential approach that can capture the
23 gas-liquid interface form directly. The finite element method

1 (Bonnerot and Jamet, 1977; Lynch, 1982) and a boundary–
2 fitted coordinate system (Ryskin and Leal, 1984a, b) are used
3 to make a calculation cell following interface modification;
4 they require reconstruction of the calculation lattice. The
5 volume of fluid (VOF) method (Hirt and Nichols, 1981),
6 which pursues the share of fluid by the Euler method, is widely
7 known. When the VOF method is applied to a complicated
8 interface and advection of bubbles, a special technique is
9 needed to prevent accumulation of the interface form error by
10 coarse graining, and what is called numerical diffusion. These
11 techniques include the donor–acceptor method (Hirt and
12 Nichols, 1981), level–set method (Osher and Sethian, 1988),
13 CIP method (Yabe and Wang, 1985), PLIC (Rider and Kothe,
14 1998), MARS method (Kunugi, 1997), and CICSAM (Ubbink
15 and Issa, 1999). These methods each have advantages and
16 disadvantages for reconstruction of the calculation cells,
17 volume conservation, and the interface reconstruction method,
18 so it is necessary to choose the optimal method according to
19 the calculation conditions.

20 The above–mentioned problems are caused by
21 discretization of cells. The particle method is a Lagrangian
22 approach that does not use a mesh and discretizes the fluid into
23 moving particles; thus, numerical diffusion does not exist in

1 essence. In the particle method, particles themselves move by
2 advection according to their mass and volume. Therefore, the
3 algorithm is simple, and each particle maintains a sharp
4 interface. The smoothed particle hydrodynamics (SPH)
5 method (Lucy, 1977) is a particle method for fluid dynamics.
6 It was originally developed for astrophysical applications and
7 was later expanded for applications in solid and fluid
8 mechanics (Monaghan, 1994). It works by dividing the fluid
9 into a set of discrete elements referred to as particles and is
10 based on integral representation of quantities and spatial
11 derivatives. The SPH method is suitable for a compressive
12 fluid under a noticeable density change. On the other hand,
13 Koshizuka and Oka (1996) proposed the moving particle
14 semi-implicit (MPS) method, which discretized the
15 incompressible Navier-Stokes equation using a Taylor series.

16 In earlier version of MPS methods, the gas phase
17 movement has been ignored and only the liquid phase has been
18 tracked as a single-phase flow (Koshizuka and Oka, 1996).
19 This avoids the numerical instability caused by a large pressure
20 gradient due to the large density difference. However, new
21 algorithms for solving a multi-density fluid directly have been
22 proposed in recent years. Das and Das (2011) proposed the
23 diffuse interface model for the SPH method to solve a high-

1 density–ratio fluid, and it is also used to explore the physical
2 parameters of such bubbly flows (Das and Das, 2013).
3 Shakibaeinia and Jin (2012) proposed the weakly
4 compressible MPS (WC–MPS) method and applied it to the
5 Rayleigh–Taylor instability problem. They compared it with
6 the VOF method and concluded that the WC–MPS method
7 provides a sharper interface. Although the density ratio of this
8 MPS method was still not large (Khayyer and Gotoh, 2013),
9 their results indicated that this method can be applied to large–
10 scale industrial processes. On the other hand, Colagrossi and
11 Landrini (2003), Grenier et al. (2009; 2013) and Szwed et al.
12 (2013) already applied the multiphase SPH model to a more
13 practical bubble flow.

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

23

1

2 **2. Numerical and experimental method**

3

4 **2.1 Governing equations of incompressible fluid flow**

5

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

$$9 \quad \frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$10 \quad \frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g} + \frac{1}{\rho} \mathbf{F}_s \quad (2)$$

11 where $\mathbf{u}$ is the velocity, t is the time, ρ is the density, p is
 12 the pressure, ν is the kinetic viscosity, $\mathbf{g}$ is the gravity, and
 13 $\mathbf{F}_s$ is the surface tension translated into a force per unit fluid
 14 volume.

15

16 **2.2 Discretization**

17

18 In the particle method, continuous fluids are represented
 19 by particles, and the behavior of the fluids is tracked by the
 20 motion of the particles. The governing equations are
 21 discretized by an MPS–based method. The interaction between

1 particle i and its vicinity j is given by a weight function of
 2 the distance between particle i and j ($r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$),
 3 which is defined as follows:

$$4 \quad w_{ij} = \begin{cases} \frac{r_e}{r_{ij}} - 1 & (r_{ij} \leq r_e) \\ 0 & (r_{ij} > r_e) \end{cases} \quad (3)$$

5 where r_e is the influence radius of the weight function. In this
 6 study, $r_e = 2.1d_p$ is assumed (Tanaka and Masunaga, 2010).
 7 Here, d_p is the particle diameter. The sum of the weight
 8 functions of neighboring particles is defined as the particle
 9 number density n (Koshizuka and Oka, 1996).

$$10 \quad \langle n \rangle_i = \sum_{j \neq i} w_{ij} \quad (4)$$

11 where $\langle \rangle$ represents the interparticle interaction. Using this
 12 formulation discretizes each differential operator in eqs. (1)
 13 and (2) in the same way as in previous reports (Natsui et al.,
 14 2012b; Kon et al., 2012, 2013).

15 The pressure gradient term is written as

$$16 \quad \langle \nabla p \rangle_i = \frac{D}{n^0} \sum_{j \neq i} \left[\frac{p_j + p_i}{r_{ij}^2} r_{ij} w_{ij} \right] \quad (5)$$

17 Here, D is the number of dimensions, and n^0 is a standard
 18 particle number density. The divergent formula for the velocity
 19 vector $\mathbf{u}$ at particle i is given by

$$\langle \nabla \cdot \mathbf{u} \rangle_i = \frac{D}{n^0} \sum_{j \neq i} \left[\frac{(\mathbf{u}_j - \mathbf{u}_i) \cdot \mathbf{r}_{ij}}{r_{ij}^2} w_{ij} \right] \quad (6)$$

The Laplacian formula is given by a weighted averaging of the distribution of a physical quantity from a particle to its neighboring particles:

$$\langle \nabla^2 \mathbf{u} \rangle_i = \frac{2D}{n^0 \lambda} \sum_{j \neq i} [(\mathbf{u}_j - \mathbf{u}_i) w_{ij}] \quad (7)$$

Here, λ is a coefficient obtained from an analytical solution.

The continuum surface force (CSF) approach model was localized to a fluid interface by applying them to fluid elements in the transition region of the interface (Morris, 2000). Surface tension is converted to force per unit volume by:

$$\mathbf{F}_s = \delta \mathbf{f}_s \quad (8)$$

where δ is a surface delta function, which peaks at the interface. For judgment of surface particles, the neighboring same phase particle number N_i is used.

$$\delta = \begin{cases} 1 & (N_i < \beta N^0) \\ 0 & (N_i \geq \beta N^0) \end{cases} \quad (9)$$

where β and N^0 are the standard neighboring particle number in an incompressible state and a coefficient for surface judgment, respectively. In the present research, $\beta = 0.85$ was assumed (Tanaka et al., 2010.). Furthermore, $\mathbf{f}_s$ is the

1 force per unit area given by the interparticle potential force
 2 model (Kondo, 2007):

$$3 \quad \langle \mathbf{f}_s \rangle_i = - \frac{2\sigma d_p^2}{\Phi_i} \nabla \phi(\mathbf{r}_{ij}) \quad (10)$$

4 where σ is the surface tension coefficient, and ϕ is the
 5 interparticle potential. It is calculated as follows:

$$6 \quad \nabla \phi(\mathbf{r}_{ij}) = (\mathbf{r}_{ij} - d_p) \quad (11)$$

$$7 \quad \Phi_i = \sum_{j \neq i, \rho(j)=\rho(i)} \phi(\mathbf{r}_{ij}) \quad (12)$$

$$8 \quad \phi(\mathbf{r}_{ij}) = \frac{1}{3} \left(\mathbf{r}_{ij} - \frac{3}{2} l_0 + \frac{1}{2} \mathbf{r}_e \right) (\mathbf{r}_{ij} - \mathbf{r}_e)^2 \quad (13)$$

$$9 \quad \nabla \phi(\mathbf{r}_{ij}) = (\mathbf{r}_{ij} - d_p)(\mathbf{r}_{ij} - \mathbf{r}_e) \quad (14)$$

10 The solid–liquid wettability is expressed quantitatively by the
 11 contact angle θ , similar to that in a previous report (Natsui et
 12 al., 2012b).

$$13 \quad \langle \mathbf{F}_s \rangle_{l-s} = \frac{1}{2} (1 + \cos \theta) \cdot \langle \mathbf{F}_s \rangle_{l-l} \quad (15)$$

14 where $l-s$ represents between liquid and solid, $l-l$
 15 represents between liquid and liquid.

16 We obtain n^0 assuming a uniform particle number
 17 density, and this is considered to represent the incompressible
 18 state. Here, $\lambda = \sum_{j \neq i} (w_{ij} r_{ij}^2) / \sum_{j \neq i} w_{ij}$. The governing

equations are discretized by using the above-mentioned operators, and the particle's equations of motion are obtained as explicit solutions.

2.3 Smoothed interface density function

In a gas-liquid two-phase flow, because the density at phase boundaries is not a steady value, ρ is newly defined as the density function of each particle.

$$\rho_i = \langle \rho \rangle_i \quad (16)$$

This means that the density of the fluid varies with the spatial distribution. The large density difference at a two-phase interface dramatically affects the momentum exchange. To smooth the pressure gradient between the gas and the liquid, a smoothed interface density function is introduced in boundary particles (Shakibaeinia and Jin, 2012).

$$\langle \rho \rangle_i = \sum_{j \neq i} m_j w_{ij} / \int_V w_{ij} dV \quad (17)$$

where m_j is the mass of the particle j , and V is the volume of the fluid. Figure 1 shows a schematic diagram of the smoothed change in the density function at the gas-liquid interface. The density function away from the gas-liquid

1 interface becomes equal to the actual fluid density.

2 3 2.4 Pressure calculation 4

5 The pressure at the next step remains unknown. The
6 pressure is solved from the particle number density in the
7 prediction step $\langle n^* \rangle_i$, which is explicitly solved using the
8 particle velocity and initial particle density as shown in section
9 2.2. The gas phase as well as the liquid phase is discretized by
10 particles in this model, and the numerical destabilization is
11 often increased owing to the very different density at the gas–
12 liquid interface. This is caused by keeping strict
13 compressibility at the interface; thus, limited compressibility
14 is assumed to stabilize the pressure at the interface. Tait’s
15 equation of state is typically used to calculate the pressure
16 explicitly (Monaghan, 1994, 2012).

$$17 \quad p_i^{k+1} = \frac{\langle \rho \rangle_i c_0^2}{\alpha} \left[\left(\frac{\langle n^* \rangle_i}{n^0} \right)^\alpha - 1 \right] \quad (18)$$

18 where c_0 is the sound speed, and α is a fitting coefficient.
19 This equation has high stability, and it can be applied to high
20 Mach number problems such as jet flow. However, this
21 algorithm essentially does not include volume conservation
22 because the use of the compressible fluid property $c_0^2 =$

1 $\partial p / \partial \rho$ is assumed. The fluid is assumed to be barotropic in
2 this equation. In particle method, if low velocity flow is
3 considered, local particle arrangement may cause numerical
4 volume change. Generally, when the Mach number is less than
5 0.3, the influence of compressive forces is negligible. At this
6 time, the density change of a flow is less than 5 %. To consider
7 chemical reactions such as the dissolution of the gas phase in
8 a metallurgical process, it is not desirable to allow numerical
9 error to disrupt the conservation of the fluid volume.

10 Therefore, in this research, the implicit equation for
11 incompressible conditions assuming constant fluid density is
12 applied. Although the volume is conserved by assuming
13 incompressibility, it is easy to produce turbulence due to the
14 pressure. To avoid pressure vibration between particles, weak
15 compressibility is incorporated into Poisson's equation
16 (Tanaka and Masunaga, 2010).

$$17 \quad \nabla^2 p_i^{k+1} = \frac{\langle \rho \rangle_i}{\Delta t} (\nabla \cdot \mathbf{u}^*) - \frac{\gamma \langle \rho \rangle_i}{\Delta t^2} \left[\left(\frac{\langle n^* \rangle_i}{n^0} \right) - 1 \right] \quad (19)$$

18 where γ is the relaxation coefficient of incompressibility. The
19 second term on the right-hand side of eq. 19 is similar to the
20 right-hand side of eq. 18. Each coefficient is essentially
21 collected in γ . Therefore, by optimizing γ , a smooth pressure
22 distribution can be calculated while minimizing changes in the

1 volume.

2 Here, eq. 19 assumes a continuous fluid with
3 incompressible flow. As shown in Fig. 1, because a smooth
4 density function $\langle \rho \rangle_i$ is specified at the gas–liquid interface,
5 it should not be given as a constant. In this model, the spatial
6 differentiation of $\langle \rho \rangle_i$ is also considered. The following
7 Poisson’s equation is proposed for MPS method.

$$8 \quad \nabla \cdot \left(\frac{1}{\langle \rho \rangle_i} \nabla p_i^{k+1} \right) = \frac{\nabla \cdot \mathbf{u}^*}{\Delta t} - \frac{\gamma}{\Delta t^2} \left[\left(\frac{\langle n^* \rangle_i}{n^0} \right) - 1 \right] \quad (20)$$

9 This formulization is also similar to that of the C–CUP method
10 (Yabe and Wang 1991), which is a stable algorithm for
11 calculating a multi–phase flow by an Eulerian approach, and a
12 convergent calculation is applied instead of an explicit
13 calculation. Thus, interfacial stability can be obtained. Similar
14 to the divergence and gradient operators, it is straightforward
15 to obtain the direct MPS representation of the Laplace operator
16 on the left–hand side of eq. (15). We propose the approximate
17 Laplacian operator with the similar form as the viscous term
18 of eq. (7).

$$19 \quad \langle \nabla \cdot \frac{1}{\langle \rho \rangle_i} \nabla p_i^{k+1} \rangle_i = \frac{2D}{n^0 \lambda} \sum_{j \neq i} \left[\frac{(p_j - p_i)}{\langle \rho \rangle_i} w_{ij} \right] \quad (21)$$

20 This approach is also used in the SPH model (Pozorski and
21 Wawreńczuk, 2002; Szewc et al., 2012); because $\langle \rho \rangle_i$ is

1 obtained by density difference with the surrounding particles
2 in this weakly compressible model, this approach could be
3 applicable also in the MPS method. This Poisson equation is
4 computed directly on particles as irregular grid. A conjugate
5 gradient method is used to solve this equation (Hestenes and
6 Stiefel, 1952).

8 2.4 Initial particle arrangement

10 To maintain the incompressibility of the fluid, a standard
11 particle number density n^0 is given from the initial
12 arrangement of uniform fluid particles.

$$13 \quad n^0 = \sum_{j \neq i} w_{ij}^0 \quad (22)$$

14 All the particles try to maintain a constant density and be close
15 to n^0 . Figure 2 shows the initial arrangements of particles.
16 When all the fluid particles are uniform, a simple cubic (SC)
17 arrangement is common. However, the filling fraction for this
18 arrangement is relatively low ($f \approx 0.52$). Fluid particles move
19 easily under a pressure gradient because discretization of the
20 particles is assumed. As a result, the number density
21 distribution can change discontinuously. This tendency
22 becomes more remarkable in a three-dimensional simulation.

Thus, we introduce the checkerboard (CB) arrangement, a uniform particle arrangement with a high filling fraction. In the CB arrangement, a denser state is assumed as the standard for a non-compressed state, and the numerical stability at a gas-liquid interface can be improved.

2.5 Artificial viscosity

In the particle method, interpenetration between particles is a problem that occurs in high Reynolds number flows. An artificial viscosity is used to avoid this interpenetration (Monaghan, 1989). This method modifies the velocity at the prediction step $\mathbf{u}^*$ when the distance between two particles becomes less than the particle diameter.

$$\mathbf{u}_i^* = \mathbf{u}_i - \frac{1}{\rho_i} \sum_{j \in J} \left[(1 + \varepsilon) \frac{\rho_i \rho_j}{\rho_i + \rho_j} \mathbf{u}_{ij}^n \right]; \quad J = \{j: r_{ij} < d_p\} \quad (23)$$

where $\mathbf{u}_{ij}^n$ is the normal part of the relative velocity between particles i and j , and ε is the collision ratio. $\varepsilon = 0.5$ was chosen by Shakibaeinia and Jin (2012). We set $\varepsilon = 0.4$ to avoid interpenetration of particle into solid wall for application to liquid-gas two phase flow. In momentum exchanges between particles, the total linear and angular momentum are preserved. Therefore, this pairwise collision algorithm does

1 not disturb the satisfaction of the momentum equation.

2 3 2.6 Calculation conditions 4

5 The calculation domain is shown in Fig. 3. Case 1 is the
6 equilibrium situation. The stability of the gas–liquid interface
7 is analyzed using this initial configuration. In this condition, γ
8 remains unknown. Tanaka and Masunaga (2010) indicated that
9 the compressibility factor in Poisson’s equation has a non–
10 negligible scale dependency. Thus, if the spatial scale becomes
11 large, the compressive effect will become relatively large.
12 Therefore, γ must be optimized in this case. We investigated
13 the influence of γ on the pressure stability and interface shape
14 change in Case 1. In Case 2, the method is applied to an actual
15 gas–liquid system. It aims to examine the rise, modification,
16 and bursting of a single bubble at the water surface. In Case 3,
17 the cube–to–sphere bubble deformation test is attempted to
18 discuss bubble pressure (section 3.5). The calculation
19 conditions are shown in Table 1. The particle diameter was
20 constant in each condition. In order to compare simulation
21 model with an experiment, we set the diameter of particles as
22 1 mm in consideration of the calculation load and spatial
23 resolution. Dissolution of the gas to liquid was ignored.

1 Although even the contact angle of same material is influenced
2 by the solid surface's physical properties, 90° was specified
3 assuming a very small influence to the bubble's behavior. The
4 programs used in this research are all original programs
5 developed by the authors. The computer codes were written in
6 Fortran90/95; they were compiled using Intel Fortran
7 Compiler Version 11.1 in UNIX and then run. To reduce the
8 calculation time, parallel processing of the program code was
9 implemented using OpenMP.

12 2.7 Experimental

14 The simulation results were verified by comparison
15 with an isometric experiment for Case 2. A schematic of the
16 experimental apparatus is shown in Fig. 4. An acrylic cube was
17 filled with distilled water up to $y = 0.070$ m in Fig. 3 (b).
18 Next, 7.24 ml of air was added through a stainless steel pipe
19 connected to a syringe. The air was trapped in a hemisphere–
20 type dumping cup (0.030 m in diameter, plastic). As a
21 nichrome rod connected to the plastic cup is rotated 180° , an
22 air bubble will rise because of buoyancy and burst on the water
23 surface. The interface modification was recorded at a speed of

6000 fps and at 512×512 pixels using a high-speed video camera (Fastcam SA3 model, Photoron Co., Ltd.).

3. Results and discussion

3.1 Sensitivity analysis of compressive parameter at gas-liquid interface and volume change

The gas-liquid interface and volume change were compared in each compressive condition in Case 1. Changes in the steady-state gas-liquid distributions at each γ value are shown in Fig. 5. Because all the fluids were simulated assuming incompressible flow, the gas-liquid distribution should strictly maintain the initial condition in Fig. 5 (a). For $\gamma = 0.1$, as shown in Fig. 5 (b), the gas-liquid interface is stable and unclear, and the phases are mixed. The gas-liquid interface shape is no longer maintained in the incompressible condition. For $\gamma = 0.01$, as shown in Fig. 5 (c), the interface remained sharp with no mixing between the gas and the liquid. Although the gas-liquid interface also remained sharp when $\gamma = 0.001$, as shown in Fig. 5 (d), the height of the upper surface of the gas phase decreased. Thus, the total fluid volume

1 decreased in this case. This volume contraction becomes more
2 remarkable for $\gamma = 0.0001$, as shown in Fig. 5 (e). The liquid
3 phase exhibited significant volume contraction but the gas
4 phase did not. Because the liquid phase is denser, the liquid
5 volume would decrease more than the gas phase under the
6 influence of gravity.

7 Figure 6 shows the change in the fluid volume for each
8 γ . The fluid volume decreases with decreasing γ , and it
9 departs from the theoretical value. Therefore, volume
10 conservation and interfacial stability are trade-offs.
11 Considering these results, we chose an optimized value of $\gamma =$
12 0.040 and used it hereafter in this research.

13 The calculated the pressure at the center of the bottom
14 is shown in Fig. 7. For $\gamma = 0.100$, the pressure tends to
15 oscillate, causing turbulence at the local gas-liquid interface.
16 For $\gamma = 0.040$, after a slight variation in the volume,
17 hydrostatic pressure was reached. This slight variation shows
18 a constant oscillating period. Thus, it represents the
19 compression and expansion between particles caused by
20 gravity. If we set $\gamma = 0.010$, the vibration amplitude
21 decreases; however, it is necessary to permit a volume
22 decrease of about 1% in that case from Fig. 6.

23

3.2 Influence of initial particle arrangement on the bubble shape

In this section, we discuss the change in the bubble shape for each initial particle arrangement in Case 2. The time change in the bubble is shown in Fig. 8. This figure represents a vertical cross section at $z = 0.040$ m. The rising of the bubble as the result of the buoyancy caused by the density difference between the gas and the liquid was successfully simulated. The height of the fluid remained in the initial condition in each arrangement; therefore, the volume was conserved with high accuracy when $\gamma = 0.040$ is used. Here, the gas–liquid interface shape reveals that the liquid particles penetrating the bubble are in the SC arrangement. Gotoh and Sakai (2006) indicated that the liquid particles that surround the surface of a gas particle may produce pressure turbulence. In the SC arrangement, even if γ is optimized, local pressure fluctuation among particles could occur owing to the lower filling fraction. On the other hand, in the CB arrangement, the interface remains sharp. The high filling fraction can avoid mixing at the interface.

To maintain a sharp interface with a large density difference, an initial arrangement with a high filling fraction is

1 effective. If the fluid density difference increases further, the
2 effect of the particle arrangement will become remarkable
3 owing to the pressure gradient. A two-dimensional simulation
4 is often applied to gas-liquid flows but almost all of them
5 exhibit three-dimensional behavior. In the particle method, to
6 evaluate the diameter of a particle d_p and the influence radius
7 r_e as a spherical potential field, the effect of the particle
8 arrangement may become large in a three-dimensional
9 simulation.

10 The quantification of the sharpness of the gas-liquid
11 interface was investigated. The sharpness can be assumed to
12 be inversely related to the contact number of gas phase
13 particles with interface liquid particles. We defined N_f as the
14 average liquid particle number in contact with liquid particles
15 around a bubble. Figure 9 shows the change in N_f with time.
16 Here, N_{f0} represents the initial value of N_f . If N_f/N_{f0}
17 decreased, the contact number between liquid and gas particles
18 increased at the gas-liquid interface, causing diffusion at the
19 interface. In the SC arrangement, a remarkable decrease in
20 N_f/N_{f0} appeared from an early stage of the calculation.
21 Mixing of gas and liquid particles was observed at $t = 0.10$ s.
22 In contrast, the CB arrangement maintained $N_f/N_{f0} > 1.0$
23 and the gas-liquid interface very sharply. The initial bubble

1 shape was spherical, and the interfacial area increased with
2 modification of the interface shape. Thus, this result is
3 physically appropriate.

4 5 6 3.3. Model verification by comparison with experimental 7 results

8
9 The previous section showed that the gas–liquid
10 interface could be calculated stably with high accuracy by
11 using the CB arrangement. This section discusses the
12 calculation validity of this model on the basis of a comparison
13 with a cold model experiment at the same scale using the
14 configuration for Case 2. Figure 10 shows snapshots of the
15 bubble behavior obtained by the simulation and the experiment
16 at various times. Although the experimental data show a two–
17 dimensional picture, it can be seen that a dome–shaped bubble
18 rose in the liquid at $t = 0.15$ s, changed at $t = 0.20$ s, and
19 burst at the water surface at $t = 0.25$ s. However, at $t =$
20 0.20 s, although the simulation result showed that the air
21 bubbles dispersed and remained in the liquid phase, the
22 gaseous phase was not distributed that much in the experiment.
23 This difference could be caused by a decrease in the accuracy

1 of the simulation due to the limited particle number available
 2 to express the disperse phase. Moreover, the minimum
 3 thickness of water covering the surroundings of a bubble may
 4 be of the order of microns. Because the formation of a thin film
 5 on the water surface is disregarded in this calculation condition,
 6 dispersion of the gas phase could have had an effect. It is
 7 difficult to represent the thin film directly because of the
 8 difference in scale between macroscopic bubble and film
 9 thickness, consequently, a new physical model should be
 10 considered. Under this condition, the Eötvös number $Eo =$
 11 $g\rho_L D^2/\sigma = 77.5$, and the Morton number $Mo =$
 12 $g\mu_L^4/\rho_L\sigma^3 = 2.5 \times 10^{-11}$; thus, the typical bubble shape is
 13 close to a spherical cap according to Grace's diagram (Grace,
 14 1973), and the experimental result is consistent with that.
 15 Detailed experimental terminal velocity U_T for air bubbles
 16 rising in distilled water are presented by Clift et al. (1978) for
 17 the ellipsoidal regime.

$$18 \quad U_T = \sqrt{\frac{2.14\sigma}{\rho D} + 0.505gD} \quad (24)$$

19 Fig.11 shows the comparison of bubble rising velocity and
 20 theoretical terminal velocity based on eq. (18). Rising velocity
 21 obtained by calculation was rather smaller than theoretical

1 terminal velocity. For an air bubble in water, there is little
2 viscous resistance to internal circulation, and hence the drag
3 and terminal velocity are sensitive to surface pressure. It is
4 suggested that the improvement of accuracy of a surface
5 tension model is important for the exact estimation of terminal
6 velocity, as section 3.5 also describes. It is an early stage of a
7 rising bubble, and it does not reach the terminal velocity.
8 However, the calculation result showed the experimental
9 bubble shape and rising velocity to be qualitatively correct.

10 The time change in the diameter of a bubble is shown in
11 Fig. 12. The tip of a bubble in the experimental data at each
12 time was analyzed using image processing software and
13 compared with the simulation results. Although the error
14 between the experimental and calculation results was
15 approximately 1–2 mm (i.e., one or two discrete particles) in
16 the bubble width D_x , the tendency was successfully predicted.
17 Although the bubble height D_y was mostly in good
18 agreement with the experimental results before the collision
19 with the top surface of the liquid, an error with a maximum of
20 about 4 mm occurred after the collision. In this experiment,
21 because the bubble shape showed a slight tendency to increase,
22 it is necessary to correctly specify the initial condition in order
23 to increase the accuracy.

3.4. Dispersed bubbles behavior

In general, VOF methods always incorporate numerical diffusion, especially at a gas–liquid interface, even if a special technique is used. Thus, volume conservation of each dispersed bubble is difficult, and the interface cannot be tracked. The greatest advantage of this model is that it allows calculating the dispersed phase directly without using the mesh. Figure 13 shows snapshots of the gas–liquid interface obtained from the simulation (Figure 13a) and from the experiment (Figure 13b) at $t = 0.34\text{s}$. Note that bubbles that are dispersed on the front side are not seen because this figure shows a vertical cross–section. The location of dispersed bubbles (about $y = 0.06$) was simulated. Therefore, this model has predicted with high accuracy the existence of a gas–liquid interface on the top surface of a liquid, and in addition it predicted the dispersed bubbles behavior. Moreover, incompressible flow was assumed in this model; thus, fluid volume was essentially conserved. However, the shapes of dispersed bubbles should be improved. Figure 14 shows the temporal change in the velocity vector distribution in a vertical cross–section. Near the gas–liquid interface, a bubble burst in

1 a whirl. The flow pattern of a bubble interior and liquid was
2 almost the same as those in conventional results (Tomiya et
3 al., 1991). On the other hand, local fluctuation is expressed by
4 each particle discrete behavior in this simulation model. This
5 model could predict dispersed bubbles that remain in the liquid
6 phase. By further improving the accuracy of this model, a
7 quantitative evaluation of the dynamic dispersed behavior is
8 expected.

9 Three-dimensional gas-liquid interfaces are shown in
10 Fig. 15. The immersed boundary method was used to visualize
11 the interfaces in this figure by applying the gas-liquid interface
12 information to sufficiently small tetragonal lattices (Ikeno and
13 Kajishima, 2007). As shown in this experiment, the behavior
14 of even a simple single bubble changes to a fully three-
15 dimensional dispersion, so we believe that just our two-
16 dimensional information in the conventional picture is
17 insufficient to predict the behavior in actual metallurgical
18 processes. In the future, this model will be an effective method
19 for predicting the disperse phase by simulating the position,
20 velocity, pressure, and other parameters of the fluid elemental
21 volume.

22 23 3.5. Model verification of flows governed by surface tension

1
2 In a gas–liquid interface, it is important to estimate the amount
3 of surface tension correctly. This model employs the inter–
4 particle potential model proposed by Kondo et al. (2007). The
5 authors attempted a droplet deformation test in the previous
6 article, and the results show good agreement with the
7 theoretical period of droplet oscillation (Natsui et al., 2012).
8 However the fundamental tests are not enough given in gas–
9 liquid direct model. Here, three–dimensional cube–to–sphere
10 bubble deformation is considered using this model. It involves
11 a cubical box of fluid with an edge of length $L = 0.052\text{ m}$, as
12 the inner gas phase, and a centered cubical volume of another
13 fluid of edges $l = 0.018\text{ m}$ as shown in Fig. 3 (c). CB
14 arrangement of particles was chosen for this simulation. The
15 calculation result is shown in Fig. 16. Because of the surface
16 tension, the initially cubic volume of the inner gas phase
17 ultimately becomes spherical in shape. The pressure inside the
18 bubble must be higher than in the surrounding liquid and
19 should represent a jump at the interface from the Young–
20 Laplace equation:

$$\Delta p = \sqrt[3]{\frac{4\pi}{3} \frac{2\sigma}{l}} \quad (25)$$

1 The steady state pressure distribution is shown in Fig. 17. In
 2 this figure, only the particles that cross a center of bubble were
 3 tracked ($y = L/2 \pm l_0$, $z = L/2 \pm l_0$). The pressure
 4 distribution was not constant in a bubble, and local fluctuation
 5 could be seen when the flow was governed by surface tension.
 6 As compared with Fig. 7, although a time pressure vibration of
 7 particles was able to keep stability by this method, a spatial
 8 vibration appeared. This model was not able to estimate
 9 surface tension between gases and liquids more accurately
 10 than the WCSPH model (e.g., Szewc et al., 2012; 2013). The
 11 pressure distribution is not smooth; nonetheless, the fluid
 12 motion was quantitatively natural. This reason is supposed as
 13 below. The fluid is compressed and the pressure is induced to
 14 be high owing to this pressure fluctuation. A repulsive force
 15 acts between particles because of high pressure, and a decrease
 16 in the fluid volume is prevented. The fluid motion is observed
 17 naturally even though the pressure is not evaluated correctly.
 18 In the future, the model for surface tension between gases and
 19 liquids should be improved for realizing a more stable multi-
 20 density interface.

21

22

23 4. Conclusion

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

A new calculation procedure for a three-dimensional direct particle simulation model of a gas–liquid flow was proposed. Because the gas phase and liquid phase are directly discretized as particles, it is practical and useful for application in actual processes. The following conclusions can be drawn from this study:

Numerical instability can occur because of the large pressure gradient among particles due to the large density difference, such as that at the gas–liquid interface. In this study, the stability of the interface was improved by introducing weak compressibility and a smooth density function in Poisson’s equation. Here, to avoid decreasing the fluid volume, a method of optimizing a compressive parameter was proposed by comparison with a theoretical hydrostatic pressure.

Moreover, a CB initial arrangement of the particles was stable instead of a conventional SC arrangement. This higher filling ratio arrangement could maintain the standard particle number density as the condition of an incompressible fluid, and it avoided the large pressure gradient at the interface. Even the bubble rising behavior could remain stable in the gas–liquid simulation when this initial arrangement was used.

The simulation model was verified by comparison with

1 a cold model experiment on the same scale. A high-speed
2 video camera was used to observe a bubble's behavior in the
3 liquid phase. This model predicted the transient shape and
4 velocity of the rising bubble with high accuracy. However,
5 because this model did not introduce a physical model to
6 represent a thin film on the water surface, the error of the
7 dispersion phase distribution was increased.

8 The gas-liquid interface was simulated with volume
9 conservation using this model as opposed to the conventional
10 MPS method. Local fluctuation of pressure of the interface has
11 been also discussed, but further studies are necessary to
12 resolve this problem. This study is an intermediate step. In the
13 future, this model can be applied to predict the outcomes of
14 actual industrial processes.

15

16

17 **Nomenclature**

18

19 Symbols:

20	d	diameter, m
21	D	dimension number, —
22	F	force, N
23	g	gravity, m/s^2

1	m	mass, kg
2	n	number density, —
3	n^0	standard number density, —
4	n^*	number density in the prediction step, —
5	N	number of surrounding particles, —
6	p	pressure, Pa
7	r	distance, m
8	$\mathbf{r}$	positional vector, m
9	t	time, s
10	$\mathbf{u}$	velocity, m/s
11	$\mathbf{u}^n$	normal part of relative velocity, m/s
12	$\mathbf{u}^*$	velocity in the prediction step, m/s
13	V	volume, m^3
14	w	weight function, —
15		
16	Greek letters:	
17	γ	relaxation coefficient of incompressibility, —
18	ε	collision ratio, —
19	λ	coefficient obtained from analytical solution, —
20	ν	kinetic viscosity, m^2/s
21	ρ	density, kg/m^3
22	σ	surface tension coefficient, N/m
23	ϕ	interparticle potential, —

1

2 Subscripts:

3 e effective

4 f fluid

5 i index of particle

6 j vicinity particle index of particle i

7 p particle

8 s surface

9

10

11 Acknowledgment

12

13 This research was supported by Advanced Low Carbon
14 Technology Research and Development Program of Japan
15 Science and Technology Agency “JST–ALCA”. And, author
16 S. Natsui was partially supported by the Mazda Foundation
17 research promotion in Japan.

18

19 References

20

21 Bird, R. B., W. E. Stewart and E. N. Lightfoot, 2006.
22 “Transport phenomena”, 2nd ed., John Wiley & Sons, New
23 York, 554–562.

1
2 Bonnerot, R., and P. Jamet, 1977. “Numerical computation of
3 the free boundary for the two-dimensional Stefan problem by
4 Space-time Finite Element”, J. Comput. Phys., **25**, 163–181.
5
6 Colagrossi, A., and M. Landrini, 2003. “Numerical simulation
7 of interfacial flows by smoothed particle hydrodynamics”, J.
8 Comput. Phys., **191**, 448–475.
9
10 Colagrossi, A., B. Bouscasse, M. Antuono, and S. Marrone,
11 2012. “Particle packing algorithm for SPH schemes”,
12 Computer Physics Communications, **183**, 1641–1653.
13
14 Clift, R., J. R. Grace, and M. E. Weber, 1978. “Bubbles, Drops,
15 and Particles”, Chapter 7, Academic Press, New York, San
16 Francisco, London, 169–202.
17
18 Das, A. K., and P. K. Das, 2011. “Incorporation of diffuse
19 interface in smoothed particle hydrodynamics:
20 Implementation of the scheme and case studies”, Int. J. Numer.
21 Meth. Fluids, **67**, 671–699.
22
23 Das, A. K., and P. K. Das, 2013. “Bubble evolution and

1 necking at a submerged orifice for the complete range of
2 orifice tilt ”, *AIChE J*, **59**, 630–642.

3

4 Gotoh, H. and T. Sakai, 2006. “Key issues in the particle
5 method for computation of wave breaking”, *Coastal*
6 *Engineering*, **53**, 171–179.

7

8 Grace, J. R., 1973, “Shapes and velocities of bubbles rising in
9 infinite liquids”, *Trans. Inst. Chem. Eng.*, **51**, 116–120.

10

11 Grenier, N., M. Antuono, A. Colagrossi, D. Le Touzé, B.
12 Alessandrini, 2009. “An Hamiltonian interface SPH
13 formulation for multi–fluid and free surface flows”, *Journal of*
14 *Computational Physics*, **228**, 8380–8393.

15

16 Grenier, N., D. Le Touzé, A. Colagrossi, M. Antuono, and G.
17 Colicchio, 2013. “Viscous bubbly flows simulation with an
18 interface SPH model”, *Ocean Eng.*, **69**, 88–102.

19

20 Han, Z., and L. Holappa, 2003. “Mechanism of iron
21 entrainment into slag due to rising gas bubbles”, *ISIJ*
22 *International*, **43**, 292–297.

23

- 1 Hirt, C. W., and B. D. Nichols, 1981. “Volume of Fluid (VOF)
2 method for the dynamics of free boundaries”, Journal of
3 Computational Physics, **39**, 201–225.
4
- 5 Hestenes, M. R. and E. Stiefel, 1952. “Methods of conjugate
6 gradients for solving linear systems”, Journal of Research of
7 the National Bureau of Standards, **49**, 409–436.
8
- 9 Ikeno, T., and T. Kajishima, 2007. “Finite–difference
10 immersed boundary method consistent with wall conditions
11 for incompressible turbulent flow simulations”, Journal of
12 Computational Physics , **226**, 1485–1508.
13
- 14 Khayyer, A. and H. Gotoh, 2013. “Enhancement of
15 performance and stability of MPS mesh–free particle method
16 for multiphase flows characterized by high density ratio”,
17 Journal of Computational Physics, **242**, 211–233.
18
- 19 Kon T., S. Natsui, S. Ueda, R. Inoue, and T. Ariyama, 2012.
20 “Numerical Simulation of Dripping Behavior of Droplet in
21 Packed Bed Using Particle Method”, ISIJ International, **52**,
22 1565–1573.
23

- 1 Kon, T., S. Natsui, S. Ueda, R. Inoue, and T. Ariyama, 2013.
2 “Influence of Physical Properties of Melt on Liquid Dripping
3 in Packed Bed Analyzed by MPS Method”, ISIJ International,
4 **53**, 590–597.
- 5
- 6 Kondo, M., S. Koshizuka, and M. Takimoto, 2007. “Surface
7 tension model using inter-particle potential force in Moving
8 Particle Semi-implicit method”, Trans JSCES, 20070021.
- 9
- 10 Koshizuka, S. and Y. Oka, 1996. “Moving-particle semi-
11 implicit method for fragmentation of incompressible fluid”,
12 Nuclear Science and Engineering, **123**, 421–434.
- 13
- 14 Kunugi, T., 1997. “Direct Numerical Algorithm for
15 Multiphase Flow with Free Surface and Interface”, Trans.
16 Japan Soc. Mech. Eng. Ser. B, **63**, 1576–1584.
- 17
- 18 Lucy, L. B., 1977. “A numerical approach to the testing of the
19 fission hypothesis”, Astronomical Journal, **82**, 1013–1024.
- 20
- 21 Lynch, D. R., 1982. ”Unified approach to simulation on
22 deforming elements with application to phase change
23 problems”, Journal of Computational Physics, **47**, 387–411.

1
2 Monaghan, J. J., 1989. “On the Problem of Penetration in
3 Particle Methods”, *Journal of Computational Physics* , **82**, 1–
4 15.

5
6 Monaghan, J. J., 1994. “Simulating free surface flows with
7 SPH”, *Journal of Computational Physics* , **110**, 399–406.

8
9 Monaghan, J. J., 2012. “Smoothed particle hydrodynamics and
10 its diverse applications”, *Ann. Rev. Fluid Mech.*, **44**, 323–346.

11
12 Morris, J. P., 2000. “Simulating surface tension with smoothed
13 particle hydrodynamics”, *International Journal for Numerical*
14 *Methods in Fluids*, **33**, 333–353.

15
16 Nakamura, T., F. Noguchi, Y. Ueda, S. Nakajo, 1988. “Floating
17 behavior of molten copper and Cu–matte in Cu–slag study on
18 interfacial phenomena in phase separation of copper smelting
19 (2nd Report)”, *J. MMIJ*, **104**, 531–536.

20
21 Natsui, S., H. Nogami, S. Ueda, J. Kano, R. Inoue and T.
22 Ariyama, 2011. “Simultaneous three–dimensional analysis of
23 gas–solid flow in blast furnace by combining discrete element

1 method and computational fluid dynamics”, ISIJ International,
2 **51**, 41–50.

3

4 Natsui, S., S. Ueda, H. Nogami, J. Kano, R. Inoue and T.
5 Ariyama, 2012a. “Gas–Solid Flow Simulation of Fines
6 Clogging a Packed Bed using DEM–CFD”, Chemical
7 Engineering Science, **71**, 274–282.

8

9 Natsui S., R. Soda, T. Kon, S. Ueda, J. Kano, R. Inoue and T.
10 Ariyama, 2012b. “Wettability Model Considering Three–
11 phase Interfacial Energetics in Particle Method”, Materials
12 Transactions, **53**, 662–670.

13

14 Natsui S., T. Kon, S. Ueda, J. Kano, R. Inoue, T. Ariyama and
15 H. Nogami, 2012c. Analysis of Heat and Mass Transfer in a
16 Packed Bed by Considering Particle Arrangement, Tetsu–to–
17 Hagane, **98**, 341–351.

18

19 Natsui S., R. Shibasaki, T. Kon, S. Ueda, R. Inoue and T.
20 Ariyama, 2013. “Effect of high reactivity coke for mixed
21 charge in ore layer on reaction behavior of each particle in
22 blast furnace”, ISIJ International, **53**, 1770–1778.

23

- 1 Osher, S. and J. A. Sethian, 1988, "Fronts propagating with
2 curvature-dependent speed: Algorithms based on Hamilton–
3 Jacobi formulations", J. Comput. Phys. **79**, 12–49.
- 4
- 5 Otake, K., H. Kinoshita, T. Kikuchi, and R. O. Suzuki, 2013.
6 CO₂ gas decomposition to carbon by electro-reduction in
7 molten salt, *Electrochimica Acta*, **100**, 293–299.
- 8
- 9 Pehlke, R. D., W. F. Porter, R. F. Urban, 1974. “BOF
10 steelmaking”, vol. 2, New York, USA, 287.
- 11
- 12 Pozorski, J. and A. Wawreńczuk, 2002. “SPH computation of
13 incompressible viscous flows”, *Journal of Theoretical and*
14 *Applied Mechanics*, **40**, 917–937.
- 15
- 16 Rider, W. J. and D. B. Kothe, 1998. “Reconstructing Volume
17 Tracking”, *Journal of Computational Physics*, **141**, 112–152.
- 18
- 19 Ryskin, G. and L. G. Leal, 1984. “Numerical solution of free–
20 boundary problems in fluid mechanics, Part1. The Finite–
21 difference technique”, *J. Fluid Mech.*, **148**, 1–17.
- 22
- 23 Ryskin, G. and L. G. Leal, 1984. “Numerical solution of free–

- 1 boundary problems in fluid mechanics, Part2. Buoyancy–
2 driven motion of a gas bubble through a quiescent liquid”, J.
3 Fluid Mech., **148**, 19–35.
- 4
- 5 Sano, M., Y. Fujita and K. Mori, 1976. “Formation of bubbles
6 at single nonwetted nozzles in mercury”, Metal. Trans. B, **7B**,
7 300–301.
- 8
- 9 Shakibaeinia, A., and Y. C. Jin, 2012. “MPS mesh–free
10 particle method for multiphase flows”, Computer methods in
11 Applied Mechanics and Engineering, **13**, 229–232.
- 12
- 13 Szewc, K., J. Pozorski, and J. P. Minier, 2012. “Analysis of the
14 incompressibility constraint in the smoothed particle
15 hydrodynamics method”, International Journal for Numerical
16 Methods in Engineering, **92**, 343–369.
- 17
- 18 Szewc, K., J. Pozorski, and J. P. Minier, 2013. “Simulations of
19 single bubbles rising through viscous liquids using Smoothed
20 Particle Hydrodynamics”, Int. J. Multiphase Flow, **50** (2013),
21 98.
- 22
- 23 Tanaka, M., and T. Masunaga, 2010. “Stabilization and

1 smoothing of pressure in MPS method by quasi-
2 compressibility”, Journal of Computational Physics, **229**,
3 4279–4290.

4

5 Ubbink, O. and R. I. Issa, 1999. “A Method for Capturing
6 Sharp Fluid Interfaces on Arbitrary Meshes”, Journal of
7 Computational Physics, **153** , 26–50.

8

9 Takewaki, H., A. Nishiguchi and T. Yabe, 1985. The Cubic-
10 Interpolated Pseudo-particle (CIP) method for solving
11 hyperbolic-type equations, Journal of Computational Physics,
12 **61**, 261–268.

13

14 Tomiyama, A., A. Sou, H. Minagawa and T. Sakaguchi, 1991.
15 “Numerical Analysis of a Single Bubble with VOF Method”,
16 Trans. Japan Soc. Mech. Eng. Ser. B, **57**, 2167–2173.

17

18 Yabe, T. and P. Y. Wang, 1991. “Unified Numerical Procedure
19 for Compressible and Incompressible Fluid”, J. Phys. Soc. Jpn.,
20 **60**, 2105–2108.

21

22

23

Fig. 1. Schematics of shape at a gas–liquid interface.
Smoothed density is used for pressure gradient calculation.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

Fig. 2. Variation of particle arrangements in different initial conditions.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

Fig. 3. Schematic diagrams of the computational domain and initial configuration.

Fig. 4. Schematic diagrams showing the experimental apparatus for verification of Case 2.

Fig. 5. Comparison of calculation results of density distribution for each compressive parameter γ of Case 1. Grey, white and black particles denote gas, liquid and solid phases, respectively ($t=0.31$ s).

Fig. 6. Fluid volume as a function of γ . V_0 represents the initial volume of the fluid.

Fig. 7. Comparison of theoretically predicted and simulated transient behaviors of pressure at the bottom.

Fig. 8. Transient behavior of a single bubble rising through liquid, for different initial arrangement conditions. Grey, white and black particles denote gas, liquid and solid phases, respectively.

Fig. 9. Temporal change of the average number of liquid phase particles around liquid–gas interface. Black and white particles denote gas and liquid phases, respectively.

Fig. 10. Comparison of experimental photographs and calculated shapes of gas bubbles rising through the water.

Fig. 11. Comparison of calculated bubble rising velocity and terminal velocity given by eq. 18. The rising velocity was calculated from the time change of the top of bubble.

Fig. 12. Comparison of calculated and experimental results for temporal evolution of spread diameters of air bubbles in water.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

Fig. 13. Comparison of experimental photograph and calculated shapes of dispersed bubbles at $t = 0.34$ s.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

Fig. 14. Velocity vector distribution on vertical cross-section for each particle ($z = 0.040$).

Fig. 15. Three-dimensional transient behavior of a single bubble rising through viscous liquid. Semi-transparent surfaces represent gas-liquid free surfaces.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23

Fig. 16. Gas phase distribution of the cubic-to-sphere deformation test: (a) the initial state and (b) the steady state.

Fig. 17. Pressure profile at the steady state of the cubic-to-sphere deformation test.

Table 1 Calculation and experimental conditions.

Time step	dt [s]	1.0×10^{-6}	
Diameter of particles	l_0 [m]	1.0×10^{-3}	
Number of particles	N_p [–]	Case 1: $20 \times 80 \times 10$ (16000)	
		Case 2: SC: $80 \times 80 \times 80$ (512000)	
		Case 2: CB: $56 \times 112 \times 112$ (702464)	

Fluid		Liquid	Gas
		Water (298 K)	Air (298 K)
Density	ρ [kg/m ³]	1000.0	1.2
Kinetic viscosity	ν [m ² /s]	1.36×10^{-6}	1.50×10^{-5}
Surface tension	σ [N/m]	7.28×10^{-2}	
Contact angle	θ [deg]	90	

Table 1

Table 1

Time step	dt [s]	1.0×10^{-6}	
Diameter of particles	l_0 [m]	1.0×10^{-3}	
Number of particles	N_p [–]	Case 1: $20 \times 80 \times 10$ (16000) Case 2: SC: $80 \times 80 \times 80$ (512000) Case 2: CB: $56 \times 112 \times 112$ (702464) Case 3: $36 \times 72 \times 72$ (186624)	
Fluid		Liquid	Gas
		Water (298 K)	Air (298 K)
Density	ρ [kg/m ³]	1000.0	1.2
Kinetic viscosity	ν [m ² /s]	1.36×10^{-6}	1.50×10^{-5}
Surface tension	σ [N/m]	7.28×10^{-2}	
Contact angle	θ [deg]	90	