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Simulations of Droplets falling on a solid surface Using Phase-Field Method

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Abstract

Due to the accident involving the Fukushima-Daiichi nuclear power plants, it becomes necessary to construct a numerical scheme to precisely evaluate the process of meltdown, including phase transformation among solid, liquid and gas phases. In this study, we constructed a model for gas-liquid two-phase flow with a high density ratio. We used the phase-field method to express a droplet of molten nuclear fuel flowing down a wall. By performing a dam break simulation using the developed model, we confirmed the model's validity. We also performed a numerical simulation of a droplet falling down a solid surface with wettability. The wettability was modeled by setting the boundary condition of the phase-field variable. As a result, we confirmed that the developed model can express the typical characteristics of a falling droplet on a wall.

Keywords: Two-phase flow, Phase-field method, Navier-Stokes equation, Contact angle, Droplet

Introduction

The development of a simulation model able to accurately evaluate the meltdown process was made urgent by the accident at the Fukushima-Daiichi nuclear power plants. This process includes phase changes, such as melting and solidification, as well as the falling down of molten material. In order to simulate gas-liquid two-phase flow including phase change, we needed to choose an interface tracking method. The volume of fluid (VOF) method (Tomiyama, Sou, Minamigawa and Sakagushi, 1991; Minato, Ishida and Takamori, 2000; Tan, Aoki, Inoue and Yoshitani, 2011) and the level-set method (Olsson and Kreiss, 2005; Tan, Aoki, Inoue and Yoshitani, 2011) are widely used as interface tracking methods for gas-liquid two-phase flow. Since the VOF method uses a sharp interface, applying it to treat complicated morphologies is difficult. The level-set method requires re-initialization of the advection equation, leading to large calculation costs. Therefore, in this study we used the phase-field method as an interface tracking method. The phase-field method has multiple advantages; it can automatically construct an interface of complex shape and express interface migration simply by solving a time evolution equation. The biggest reason for applying the phase-field method in this study is that it enabled the expression of phase changes among gas, liquid and solid states using the multi-phase-field method. The purpose of this study was to construct the gas-liquid two-phase flow model which can express a falling droplet on a wall using the single phase-field method.

Numerical model and calculation technique

Governing equations of the two-phase flow model

In this study, we constructed a model to simulate gas-liquid two-phase flow with a high density ratio in order to express droplets falling on a solid surface. The phase-field method was used as an interface tracking method and was coupled with the Navier-Stokes equation for incompressible flows. In phase-field method, we used the Cahn-Hilliard equation with an advection term of conservation form, where the phase-field variable ϕ was regarded as a conserved quantity to keep a constant liquid volume. The phase-field variable ϕ was defined as 0 in the gas phase and 1 in the liquid phase, and it continuously and sharply changed from 0 to 1 in the interface region. The Navier-Stokes equation includes surface tension force and gravity force terms, considered body force in previous work (Anderson, McFadden, and Wheeler, 1998; Inamuro, Ogata, Tajima and Konishi, 2004; Takada, Matsumoto, Matsumoto and Ichikawa, 2008; Borcia, Borcia and Bestehorn, 2006; Borcia and Bestehorn, 2007). The governing equations of the gas-liquid two-phase flow model are

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \vec{u}) = -M_\phi \nabla^2 \eta$$

$$\eta = a^2 \nabla^2 \phi + W\phi(1-\phi)\left(\phi - \frac{1}{2}\right) \tag{1}$$

$$\nabla \cdot \vec{u} = 0 \tag{2}$$

$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u}\right) = -\nabla p + \mu \nabla^2 \vec{u} + \phi a^2 \nabla \nabla^2 \phi + (\rho_v - \rho)\vec{g}\ , \tag{3}$$

where $\vec{u}$ denotes the velocity vector; M_ϕ, phase-field mobility; η, chemical potential; a, the gradient coefficient; W, the energy barrier; ρ, density; p ,pressure; μ, viscosity; and $\vec{g}$, the gravitational acceleration vector. The gradient coefficient a and energy barrier W are related to physical properties by the following equations.

$$a = \sqrt{\frac{3\delta\gamma}{b}} \tag{4}$$

$$W = \frac{6\gamma b}{\delta} \tag{5}$$

Here, δ denotes interface width; γ, the interface energy between gas and liquid; and b, the coefficient to be related to the interface ($b \approx 2.2$). We assumed that the density ρ and viscosity μ continuously changed in the interface region, with a change in the phase-field variable, according to following equations.

$$\rho = \rho_l \phi + \rho_v (1-\phi) \tag{6}$$

$$\mu = \mu_l \phi + \mu_v (1-\phi) \tag{7}$$

The subscripts v and l represent the gas and liquid phases, respectively.

Numerical scheme

The Cahn-Hilliard equation was solved by a perfectly explicit method. The Laplacian discretization of the phase-field variable and chemical potential was evaluated with a fourth-order central difference scheme. The advection term was evaluated with a third-order upwind scheme. Time integration was evaluated with a first-order forward difference scheme. The solution of the flow field was obtained using the SMAC method. The Poisson equation for pressure was discretized by a second-order scheme and the sparse matrix was solved using the SOR method. The diffusion term was evaluated with a second-order central difference scheme. The advection term and the time integration were calculated with the same scheme as the Cahn-Hilliard equation.

Dam break problem

The dam break problem is well-known for validity verification of gas-liquid two-phase flow calculation code. Therefore, in this study we confirmed the reliability of our calculation code using a two-dimensional calculation of this problem. The computational model of a water-air system is shown in Figure 1. The initial water column width a and height $n^2 a$ were $a = 57.15 \times 10^{-3}$ m and $n^2 a = 114.3 \times 10^{-3}$ m (aspect ratio $n^2 = 2$); the same values were used in a previous experiment by Martine and Moyce (Martine and Moyce, 1952). The physical properties were as follows $\rho_l = 1000\ \mathrm{kg/m^3}$, $\mu_l = 1.137 \times 10^{-3}\ \mathrm{Pa \cdot s}$, $\rho_v = 1.226\ \mathrm{kg/m^3}$, $\mu_v = 1.78 \times 10^{-5}\ \mathrm{Pa \cdot s}$, $\gamma = 72.8 \times 10^{-3}\ \mathrm{J/m^2}$, $\delta = 4\Delta x$ and

$M_\phi = 1.0\times10^{-4}$ m^5/(J·s). The lattice number was set to 160×160. The lattice sizes, Δx and Δy, and the time increment Δt were $\Delta x = \Delta y = 1.43\times10^{-3}$ m and $\Delta t = 1.05\times10^{-6}$ s. In all boundaries, we set the following conditions: $\vec{n}\cdot\nabla\phi = 0$, $\vec{n}\cdot\nabla\eta = 0$, $\vec{n}\cdot\vec{u} = 0$ and $\vec{n}\cdot\nabla p = 0$, where $\vec{n}$ denotes the normal vector. Equation (8) represents a static contact angle of 90 degrees and Equation (9) represents the fact that fluids cannot pass through the wall boundaries.

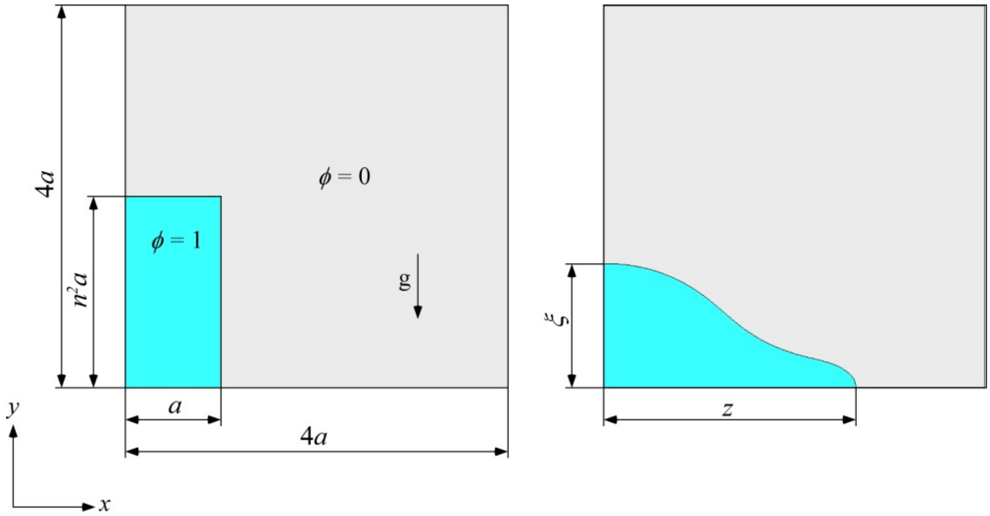
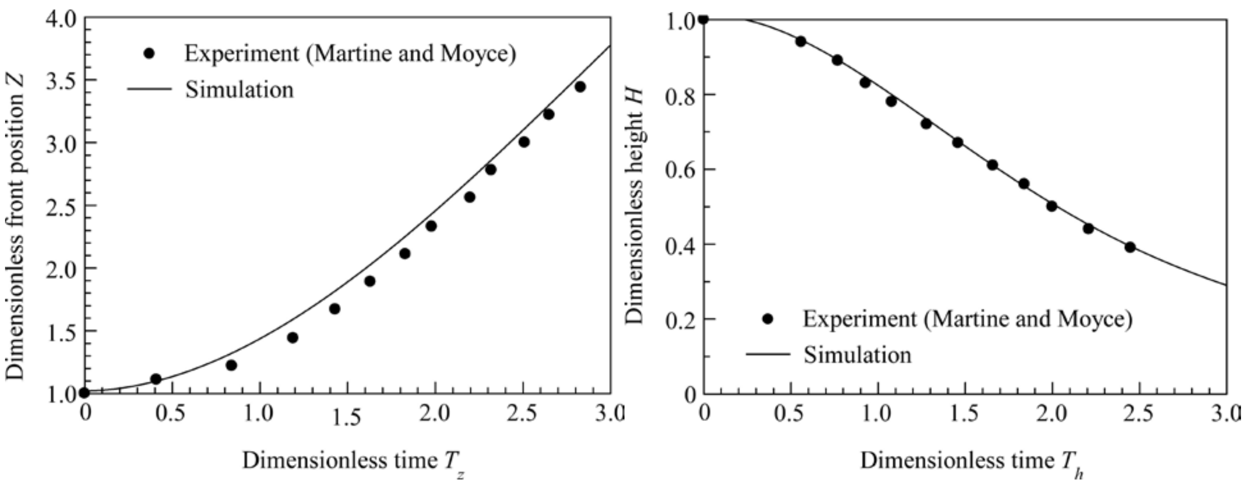


Figure 1. Computational model for the dam break problem.

Time variations of the front coordinate z and height ξ when the water column is broken by the gravity force are shown in Figure 2. Here, z, ξ and respective times are nondimensionalized by $Z = z/a$, $T_z = nt\sqrt{g/a}$, $H = \xi/(n^2a)$ and $T_h = t\sqrt{g/a}$.

As shown in Figure 2(a), the front position moved more rapidly in the simulation than in the experiment. This is because the experiment was not perfectly two-dimensional even though it was performed in a thin region of the thickness dimension. In addition, the initial rectangular water column and its sudden breaking were difficult to express in the experiment. In Figure 2(b), the time variation of the height corresponds faithfully. Although there are some discrepancies between the numerical and experimental results, we see reasonable agreement between them and can thus confirm the reliability of our calculation code.



(a) front (b) height

Figure 2. Time variations of front and altitudinal contact lines in the dam break problem.

Droplet falling on a solid surface with wettability

Boundary conditions for wettability

In order to give wettability to the boundary, we introduced an idea which implements the geometry shown in Figure 3. This model is different from that used in previous work (Briant, Papatzacos and Teomans, 2002); it directly gives wettability to the boundary. The contact angle θ formed by the interface energy between solid and liquid and between liquid and gas (black vectors in Figure 3) is geometrically identical to the angle formed by the normal vector $\vec{n}$ of the wall and the outward interfacial normal vector $-\nabla\phi$ (red vectors in Figure 3). Then, by calculating the inner product of the two red vectors, the boundary condition giving wettability to the left boundary is given by the following equation.

$$\frac{\partial\phi}{\partial x} = \pm\sqrt{\frac{\cos^2\theta}{1-\cos^2\theta}}\left|\frac{\partial\phi}{\partial y}\right| \quad \begin{cases} \text{if } \cos\theta < 0 \text{ then sign is } + \\ \text{otherwise, sign is } - \end{cases} \tag{16}$$

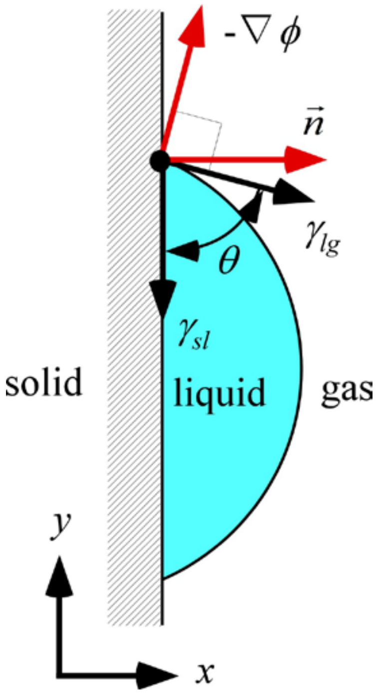


Figure 3. Boundary condition of wettability.

Numerical conditions and results

We conducted the numerical simulation of a droplet falling down a solid surface with wettability. The leftmost part of Figure 4 shows the computational domain and initial condition. The velocity of the initial semicircular droplet was set to zero. The boundary condition of the phase-field variable on the left wall was set to the Neumann condition considered wettability given by Equation (16).We set the contact angle to $\theta = 70$ °. The other boundary conditions were identical to those used for the simulation of the dam break problem in the previous section. The other parameters were also unchanged from the previous simulation, with the following exceptions: $M_\phi = 5.0\times10^{-7}$ $\mathrm{m^5/(J\cdot s)}$, $\Delta x = \Delta y = 5.0\times10^{-5}$ m and $\Delta t = 8.99\times10^{-9}$ s.

Figure 4 shows the morphological changes of a droplet on a solid surface with wettability. The upper part of the droplet becomes thin and the lower part expands as time progress. The bottom and side of the droplet become flat. In the simulation, we assumed phase-field mobility. If we used a larger value, the droplet shape would tend to be round due to the influence of curvature. To perform quantitative simulation, we needed to accurately identify the value of phase-field mobility. Time variations of advancing and receding contact angles are shown in Figure 5. In the early stage of falling, the contribution from the boundary condition is larger than that from the gravity force. Therefore, the advancing and receding contact angles approached the static contact angle $\theta = 70$ °. With time, because the contribution from the gravity force became larger, the advancing contact angle increased and the receding contact angle decreased to minimize the system energy.

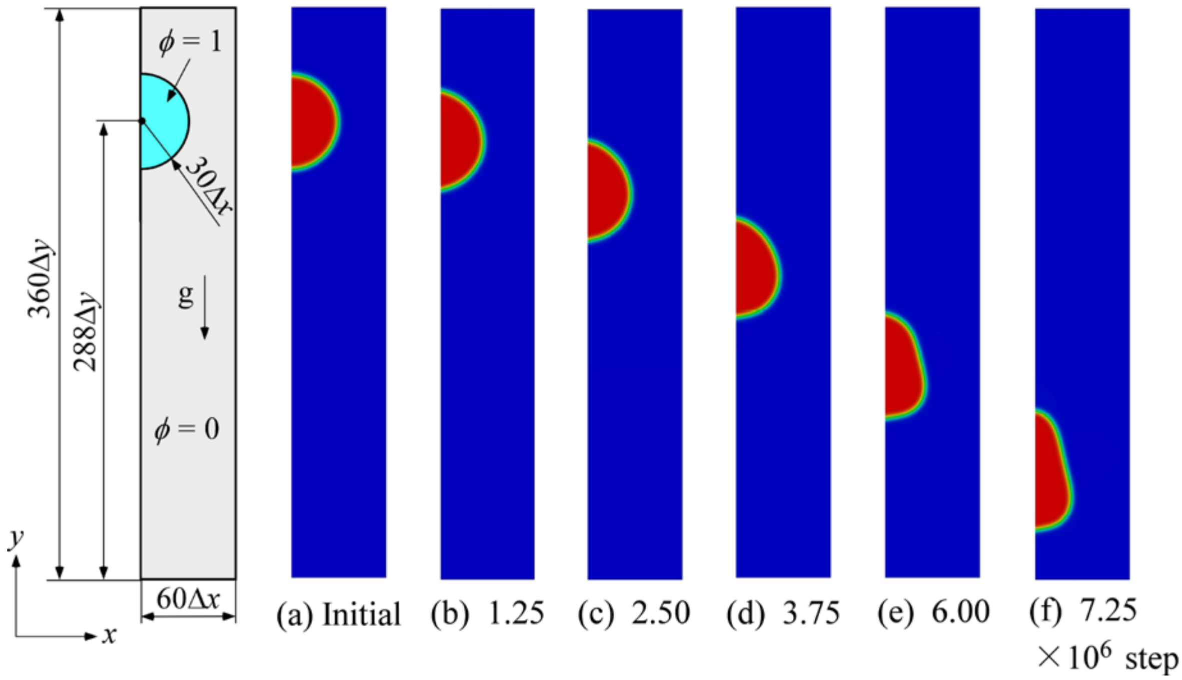


Figure 4. Computational domain and morphological changes of droplet on a wall surface with wettability.

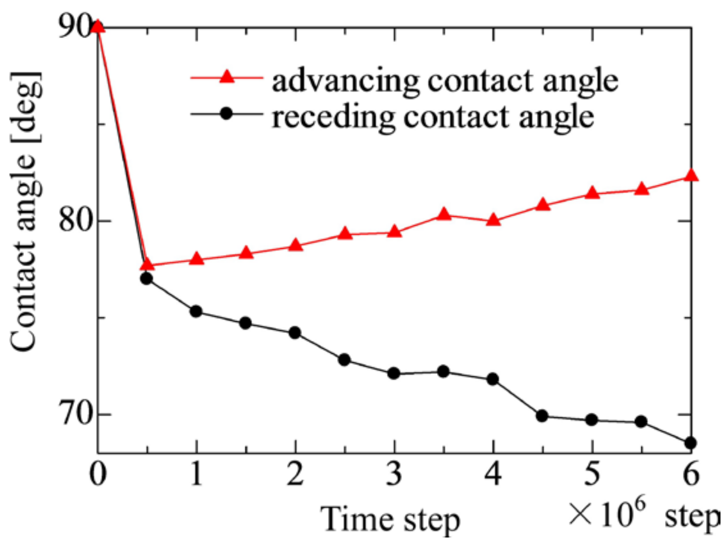


Figure 5. Time variations of advancing and receding contact angles.

Conclusions

We constructed a model for gas-liquid two-phase flow with a high density ratio by using the phase-field method. Using the two-dimensional dam break problem, we confirmed that our calculation code can reasonably simulate gas-liquid two-phase flow with a high density ratio. Next, we conducted a simulation of a droplet falling down a solid surface with wettability, where the wettability was modeled by setting the boundary condition of the phase field variable. It was observed that advancing and receding contact angles are changed by the contributions of the boundary condition and the external force.

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