Numerical analysis of two-phase fluid flows using a diffuse-interface model

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Abstract: A computational-fluid-dynamics method solving Navier-Stokes equations and adopting a diffuse-interface model (DIM) is applied to several isothermal or thermal two-phase flow problems. In the DIM, utilizing the free-energy approach for a non-equilibrium mesoscopic system, a fluid-fluid interface is assumed as an artificially-enlarged finite volumetric zone across which the physical properties vary continuously. The major findings from the simulations are as follows: (1) the DIM method predicts well the capillarity-driven motion of a gas-liquid interface in comparison with the theoretical predictions; (2) the method captures displacement and breakup of single liquid drop attached on solid walls caused by heterogeneous wettability; (3) it also predicts well qualitatively two-dimensional single bubble migration under a linear temperature gradient and no gravity caused by heterogeneous surface-tension force. These results prove that the DIM is one of useful fluid-fluid interface models for numerically analyze the two-phase fluid flows.

1. Introduction

Many kinds of thermo-fluidics devices with microscopic channels and cavities have recently attracted much attention of many people in a various fields of science and engineering, such as biological and chemical total analysis systems separating and mixing multiple fluids at ultra-small volume flow rate, heat pipe for cooling electronic devices, and energy-efficient flexible thin-film display (Berthier et al. 2006). For optimizing such devices to control the microscopic fluid motions, computational fluid dynamics (CFD) simulations help us well understand and predict the fluid phenomena. In this study, we apply a CFD method adopting a diffuse-interface model (DIM) utilizing the free-energy theory (Cahn & Hilliard 1958, van der Waals 1979) to several two-phase flow problems, for preliminarily examining their basic capability to simulate the fluid motions in the devices. In the DIM, a fluid interface is described as a finite volumetric zone across which physical properties vary steeply and continuously. The surface tension of the interface is defined as the increase in energy per unit area due to the local gradient of a so-called order parameter (e.g. density or concentration). The contact angle between solid-liquid and gas-liquid interfaces is obtained from the wetting potential of the solid surface through a simple boundary condition of the gradient of the order parameter on the surface. Consequently, the DIM simplifies interface- tracking calculation by using standard numerical techniques alone, and without any elaborating algorithms for the advection and reconstruction of interfaces and the evaluation of surface force in other methods (Kothe 1998). The DIM also enables us more easily predict the interface displacement in the flows with phase change where heat and mass transfer takes place across the interface (Anderson et al. 1998).

2. CFD method based on the DIM

The DIM-based CFD method for incompressible immiscible two-phase flows with high density ratio (Inamuro et al. 2004, Takada & Tomiyama 2006) solves a set of mass and momentum conservation equations, plus an advection-diffusion equation governing time evolution of the interfacial profile (Kim 2005, Matsumoto & Takada 2008),

\[ \nabla \cdot \mathbf{u} = 0, \]

\[ \rho (\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{T}, \]

\[ \partial_t \varphi + \nabla \cdot \left[ \varphi \mathbf{u} - \Gamma \varphi \nabla \left( \partial_t \varphi - \kappa \nabla^2 \varphi \right) \right] = 0, \]

where the continuous scalar variable \( \varphi \) is an index to describe the interface profile with a given width \( \kappa \).

The reversible stress tensor \( \mathbf{P} \) is expressed as follows (Anderson et al. 1998, Jamet et al. 2002).

\[ \mathbf{P} = \left( \rho - \kappa \right)^2 \nabla^2 \rho - \kappa \nabla \rho \otimes \nabla \rho, \]

where the direction of \( \xi \) axis is normal to a flat interface.

Eqs. (1)–(3) are solved by using the following conventional standard techniques (Takada et al. 2006 &2008). The three-dimensional space is discretized uniformly by using unit cubic cells on a fixed structured grid with a mesh width \( \Delta x = \Delta y = \Delta z = 1 \) in the Cartesian coordinate system \( (x, y, z) \), where the scalar and vector variables are located in a staggered arrangement. The advancement in time \( t \) is based on the second-order Runge-Kutta’s scheme for constantly increasing \( \Delta t \). The velocity \( \mathbf{u} \) and pressure \( p \) are obtained at each time step from Eqs. (1) and (2) by using the projection algorithm.

A wetting condition on a solid surface in the flow is incorporated into the DIM method through,
\[ \mathbf{n} \cdot \kappa \nabla \phi = -\gamma_s, \]  
\[ \text{(6)} \]

where \( \mathbf{n} \) is the unit vector normal to the boundary. The equation (6) is derived from a surface energy increase \( -\gamma_s \) per unit area with a parameter \( \gamma_s \) (Briant et al. 2002, Yoshino & Mizutani 2006, Takada et al. 2008).

3. Numerical results

3.1. Static contact-line problem under gravity

After investigating relationship between the static contact angle \( \theta_l \) and the parameter \( \gamma_s \), the capillary force was examined by conducting two benchmark tests for static two-phase fluid problems under gravity \( g \) (Takada et al. 2008). The first test was for the formation of a 2D liquid column between parallel vertical plates. The gas and liquid phases were assumed to be air and water under normal gravity, respectively. The width \( d \) of 32 cubic cells was equivalent to 5 mm in the actual fluid system. The test was conducted by using the following parameter values: \( |g| = 2 \times 10^3 \), \( \mu_l = 1.3 \times 10^{-4} \), \( \mu_w = 9.56 \times 10^{-3} \), \( \rho_l = 1.247 \times 10^3 \), \( \rho_w = 1.0 \) and \( \sigma = 0.620 \). As shown in Fig.1, the numerical result of the height \( h \) in each case of \( \theta_l \) agrees well with the theoretical prediction.

![Figure 1](image1.jpg)

Figure 1. Height of 2D liquid column between plates

3.2. 2D capillarity-driven two-phase flows

The DIM method was applied to the CFD simulation of motions of a two-phase fluid between parallel plates with hydrophilic surfaces under no gravity. The fluid was assumed to be an air-water system with density and viscosity ratios \( \rho_l/\rho_w = 801.7 \) and \( \mu_l/\mu_w = 73.76 \), respectively, in the gap space of 5 mm.

![Figure 2](image2.jpg)

Figure 2. Snapshots of the liquid permeating the gap

Figure 2 shows time series of the profiles of the liquid phase between the plates for \( \theta_l = 61^\circ \) and \( 56^\circ \). The liquid penetrates faster for smaller \( \theta_l \). The numerical result of time history of the dimensionless interface position \( s^* \) at time \( t^* \) agrees well with the theoretical prediction (Ichikawa et al. 2004) for each value of \( \theta_l \) (see Fig.3).

![Figure 3](image3.jpg)

Figure 3. Time history of the fluid interface position

3.3. 3D drop motion on partially-wetted surface

The third application is to motions of a single liquid drop on a flat solid surface in a stagnant gas under no gravity in 3D (Takada et al. 2008). This simulation was conducted for preliminarily examining the capability of the method to predict the motions of fluid particles in micro devices that control them at high frequency by a so-called electro-wetting technology. The computational domain was discretized with 64\times64\times32 cells and surrounded with stationary flat solid walls. At the center on the bottom wall, a liquid drop was initially formed with a hemisphere shape with radius equivalent to \( R=16 \) cells in the stagnant gas. The hydrophilic regions of \( \theta_{l2} \) were located on both sides of the hydrophobic one with \( \theta_{l1} \) and width \( a=R \) on the central part of the wall surface.

![Figure 4](image4.jpg)

Figure 4. Breakup of the drop on a solid surface

Figure 4 shows the time series variation in the drop shape, the interfacial profile and the flow velocity distribution on a vertical cross section in the case of \( \theta_{l1} =119^\circ \) and \( \theta_{l2}=61^\circ \) at \( t^*=1.7 \times 10^{-3} \). The Ohnesorge number \( Oh = \mu_l/\sqrt{\sigma \rho_l R} \) = 1.7 \times 10^{-3} corresponds to that of a water drop with \( R=8 \) mm in air. The result of breakup of the drop is well predicted qualitatively in comparison with the experimental observation and other numerical results (Berthier et al. 2006, Yan & Zu 2007).

3.4. Bubble migration due to Marangoni effect

For simulating a two-phase fluid motion caused by thermo-capillary force under no gravity, Eqs. (1)-(3) were solved with an advection-diffusion equation on fluid
temperature $T$. The surface tension was assumed to be decreased inversely with $T$ according to the Marangoni effect (Borcaia&Bestehorn 2002). The 3D domain was divided with $110 \times 7 \times 146$ cubic cells and surrounded with periodic boundaries in the $y$ direction and non-slip walls in the others. The Marangoni, Prandtl and Weber numbers were set at 452, 91.5 and 0.021, respectively. The numerical result of migration of the 2D bubble with diameter $d=20$ cells towards high $T$ region (Fig. 5) agrees qualitatively well with available data (Ohira et al. 2007).

![Figure 5. A snapshot of the bubble migration under VT](image)

4. Conclusions

In this study, a noble computational fluid dynamics method adopting the diffuse-interface model (DIM) and solving the Navier-Stokes equations was applied to several two-phase fluid flow problems. The major findings from the CFD simulations are as follows: (1) the DIM method predicts quantitatively well the capillary force in both of static and dynamic contact-line problems of a gas-liquid system (air-water) with a high density ratio between parallel plates in comparison with the theoretical data; (2) the method captures motions of displacement and breakup of single liquid drop on partially-wetted solid surface; (3) it also predicts well qualitatively 2D single bubble migration under a temperature gradient caused by heterogeneous surface tension force. These results prove that the DIM method will be useful for preliminarily simulating the two-phase flows in design of various thermo-fluidics devices with micro channels and cavities.

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