Numerical Simulation of Microscopic Two-Phase Flows Using Diffuse-Interface Model Based on Free-Energy Theory

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Abstract: Two versions of a computational-fluid-dynamics method solving Navier-Stokes equations and adopting a diffuse-interface model (DIM) are applied to several microscopic isothermal or thermal two-phase flow problems. In the DIM, based on the free-energy theory, a fluid interface is described as a finite volumetric zone across which the physical properties vary continuously. The major findings from the simulations are as follows: (1) the first version predicts quantitatively well the capillary force in static and dynamic two-phase fluid systems with a high density ratio (air-water); (2) the method captures displacement and breakup of liquid drops on solid walls caused by heterogeneous wettability; (3) it also predicts well qualitatively 2D single bubble migration under a linear temperature gradient caused by heterogeneous surface tension force; and (4) The second version successfully captures the van-der-Waals fluid motions with phase change around a critical point. These results prove that the DIM is one of useful interface models for simulating the flows in various micro-fluidics devices.

Many kinds of thermo-fluidics devices with micro channels and cavities have recently attracted much attention of 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 bright 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 two versions of a new CFD method adopting a diffuse-interface model (DIM) based on the van der Waals, Cahn-Hilliard 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 finite-difference 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 velocity in the flows with phase change where heat and mass transfer takes place across the interface between the phases (Anderson et al. 1998).

The first version of the DIM-based CFD method proposed for immiscible, incompressible two-phase flows with high density ratio (Takada et al. 2006) solves a set of mass and momentum conservation equations, in addition to an advection-diffusion equation governing time evolution of the interfacial profile (Jacqumin 1999, Inamuro et al. 2004, Kim 2005),

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}\right) = -\nabla \cdot \mathbf{P} + \nabla \cdot \boldsymbol{\tau}, \tag{2}$$

$$\partial_t \phi + \nabla \cdot \left[\phi \mathbf{u} - \Gamma \phi \nabla (\partial_\phi \psi - \kappa_\phi \nabla^2 \phi)\right] = 0, \tag{3}$$

In Eq.(3), the continuous scalar variable ϕ is an order parameter to describe the diffusive interface profile. The function ψ double-well on ϕ is the van-der-Waals free energy (Teng et al. 2000). κ_ϕ is a parameter to control interfacial thickness. The mobility factor Γ>0 is set to be constant. Inside the interface, the density ρ is defined as a sine-curve function of ϕ and varies between given constants ρ_G and ρ_L of gas and liquid phases. The viscosity μ in the Newtonian stress tensor $\boldsymbol{\tau}$ varies between given constants μ_G and μ_L as a function of ρ.

The reversible tensor $\mathbf{P}$ is expressed as follows.

$$\mathbf{P} = \left(p - \kappa_S \rho \nabla^2 \rho - \kappa_S \left|\nabla \rho\right|^2 / 2\right) + \kappa_S \nabla \rho \otimes \nabla \rho \tag{4}$$

p is the pressure in homogeneous field. The parameter κ_S is determined from the definition of surface tension σ (Anderson et al. 1998),

$$\sigma \equiv \kappa_S \int_{-\infty}^{+\infty} \left(\partial_\xi \rho\right)^2 d\xi , \tag{5}$$

where the direction of ξ is normal to a flat interface.

Eqs.(1)–(3) are solved by using the following conventional techniques (Takada et al. 2006, 2007 &2008). The three-dimensional space is discretized uniformly by using unit cubic cells on a fixed structured grid with 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 Δt. The velocity **u** and pressure p are obtained at each time step from Eqs. (1) and (2) by using the projection algorithm.

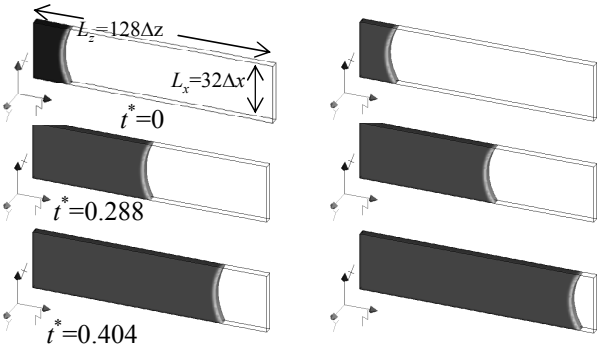
A wetting boundary condition on a solid surface in the flow is incorporated into the DIM method through,

$$\mathbf{n} \cdot \kappa_\phi \nabla \phi = -\gamma_S , \tag{6}$$

where **n** is the unit vector normal to the boundary. The equation (6) is derived from an energy increase $-\gamma_S \phi$ per unit area with a wetting potential γ_S (Briant et al. 2002, Yoshino & Mizutani 2006, Takada & Tomiyama 2007).

In this study, for simulating a gas-liquid motion caused by temperature gradient, Eqs. (1)-(3) are solved with an advection-diffusion equation on fluid temperature T. The surface tension is assumed to be decreased inversely with T according to the Marangoni effect (Borcia & Bestehorn 2002).

The second version of the DIM-CFD method for compressible two-phase flows adopts a full set of the Navier-Stokes equations with the van-der-Waals equation of state p for a non-ideal fluid (Jamet et al. 2002, Seta & Okui 2006). The order parameter is the fluid mass density ρ. They are solved by using the MacCormack finite difference scheme of second order in both of space and time plus artificial viscosity, for simplicity and stability (Takada & Tomiyama 2007).



(a) θ_W =61˚ (b) θ_W =56˚

Figure 1. Snapshots of a liquid permeating a gap between parallel plates (5mm in air-water system)

Figure 1 shows a numerical result of dimensionless-time (t^*) series of 3D profiles of a liquid phase between parallel plates under no gravity for contact angle θ_W=61° and 56°. The liquid penetrates faster for smaller θ_W.

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