Numerical Simulation of Motions of Incompressible Two-phase Fluid on Solid Surface Using a Phase-field Method

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Abstract

In this study, a phase-field method adopting Navier-Stokes equations, NS-PFM, is applied to fluid dynamic problems for examining the fundamental capability to simulate motions of incompressible isothermal two-phase fluid in various micro devices. The interfacial modeling is based on the van der Waals-Cahn-Hilliard free-energy theory. Wettability of solid surface is taken into account through a simple boundary condition derived from free-energy increase per unit area on the surface. The numerical simulations are carried out at a high density ratio equivalent to that of air-water system under no gravity. Major findings are as follows: (1) Static contact angle of liquid drop on solid surface is flexibly controlled by a parameter of wetting potential in the boundary condition. (2) Interfacial motion of two-phase fluid in a rectilinear channel is accelerated locally on a hydrophilic region of the solid surface. (3) NS-PFM successfully captures displacement and breakup motions of single liquid drop on a flat solid wall caused by difference between capillary forces on the hydrophilic and hydrophobic surfaces.

Introduction

Recently, much attention has been paid to many kinds of micro-fluidics devices with channels and cavities, such as biological and chemical micro total analysis systems (µ-TAS) (Northrup et al 2003) separating and mixing multiple fluids at ultra-small volume flow rate (Matsumoto & Tai 2004), heat pipe for cooling electronic devices (Wang & Peterson 2005), and energy-efficient bright display based on electrowetting-on-dielectric (EWOD) technology (Berthier et al 2006, Feenstra et al 2006). In optimizing device performance for accurate and flexible control of the microscopic fluid motions, numerical simulations are carried out to understand and predict the complex micro fluid phenomena in the devices, because it is difficult to observe them experimentally.

The purpose of this study is therefore to develop basic CFD codes based on a new kind of numerical method for two-phase flows, called as Navier-Stokes phase-field method (NS-PFM) hereafter, combining NS equations with phase-field modeling for interface (Anderson et al 1998, Badalassi et al 2003, Jamet et al 2001&2002, Nadiga & Zaleski 1996). Except for basic equations and numerical schemes, NS-PFM we have used (Takada et al 2005, 2006 a-d) is macroscopically equivalent to an isothermal two-phase lattice-Boltzmann method (LBM) (Inamuro et al 2004). In the phase-field modeling, based on the free-energy theory (van der Waals 1979, Cahn & Hilliard 1968), an interface is described as a finite volumetric transition zone across which physical properties vary steeply and continuously. Surface tension is given as an excessive energy per unit area caused by a local gradient of density or molar concentration. In addition, a wetting potential of solid surface yields a contact angle between solid-liquid and gas-liquid interfaces through a simple boundary condition for the order parameter on the solid surface (Briant et al 2002, Seppecher 1996, Yoshino & Mizutani 2006). The phase-field modeling, consequently, simplifies interface- capturing and tracking calculation by use of standard finite-difference techniques without any elaborating algorithms for advection and reconstruction of interfaces and evaluation of surface tension force in other conventional CFD methods (Kothe 1998).

In the previous study, the proposed NS-PFM (Takada et la 2005&2006a-d) was applied to several two-phase flow problems at high density ratio of about 800. From the numerical results, the following findings were obtained: (1) The volume flux driven by a local chemical potential gradient in the CH equation plays an important role in (a) volume conservation, (b) self-organizing reconstruction of gas-liquid interface, and (c) reduction of numerical diffusion and oscillation. (2) The method gives good predictions of pressure increase inside a bubble caused by the surface tension force. (3) Collapse of two-dimensional liquid column under gravity was predicted in good agreement with well-known experimental and numerical data. (4) Single liquid drop falling through a stagnant gas and merging into a stagnant liquid film was simulated sufficiently in three dimensions.

In this study, for examining the fundamental applicability of the NS-PFM to micro-fluidics simulations,
we propose a wetting boundary condition on solid surface in two-phase flow with high density ratio, and conduct three- dimensional numerical simulation of motions of an incompressible isothermal two-phase fluid on solid wall under gravity. The density ratio is set to be equivalent to that of an actual air-water system. In this paper, we first explain the NS-PFM and the wetting boundary condition on solid surface. The next section shows the numerical results of static contact angle of liquid drop, two-phase flows in a micro channel, and motions of single liquid drop on flat solid wall surface with heterogeneous wettability. Several conclusions are described in the last section.

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$A$</td>
<td>long-range attraction between van-der-Waals fluid particles</td>
</tr>
<tr>
<td>$a$</td>
<td>width of hydrophilic or hydrophobic region on solid surface</td>
</tr>
<tr>
<td>$B$</td>
<td>short-range repulsion between van-der-Waals fluid particles</td>
</tr>
<tr>
<td>$Ca$</td>
<td>capillary number</td>
</tr>
<tr>
<td>$I$</td>
<td>second-rank isotropic tensor</td>
</tr>
<tr>
<td>$n$</td>
<td>unit normal vector on surface of solid wall</td>
</tr>
<tr>
<td>$Oh$</td>
<td>Ohnesorge number</td>
</tr>
<tr>
<td>$P$</td>
<td>pressure tensor including surface-tension effect</td>
</tr>
<tr>
<td>$p$</td>
<td>pressure in homogeneous system</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$T$</td>
<td>parameter of free-energy function</td>
</tr>
<tr>
<td>$u$</td>
<td>flow velocity vector</td>
</tr>
<tr>
<td>$x,y,z$</td>
<td>indices of Cartesian coordinate system</td>
</tr>
</tbody>
</table>

**Greek letters**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$\Delta t$</td>
<td>time step width</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>mobility on index function $\phi$</td>
</tr>
<tr>
<td>$\gamma_S$</td>
<td>wetting potential of solid surface</td>
</tr>
<tr>
<td>$\phi$</td>
<td>index function to indicate interfacial profile</td>
</tr>
<tr>
<td>$\eta$</td>
<td>chemical potential on index function $\phi$</td>
</tr>
<tr>
<td>$\kappa_S$</td>
<td>surface tension parameter</td>
</tr>
<tr>
<td>$\kappa_d$</td>
<td>interfacial thickness parameter</td>
</tr>
<tr>
<td>$\mu$</td>
<td>viscosity of fluid</td>
</tr>
<tr>
<td>$\theta_{lw}$</td>
<td>contact angle of liquid on solid surface</td>
</tr>
<tr>
<td>$\rho$</td>
<td>mass density of fluid</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>surface tension (surface free energy/unit area)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>viscous stress tensor for Newtonian fluid flow</td>
</tr>
</tbody>
</table>

**Subscripts**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$G$</td>
<td>gas phase</td>
</tr>
<tr>
<td>$L$</td>
<td>liquid phase</td>
</tr>
</tbody>
</table>

**Superscripts**

- * dimensionless value

**Navier-Stokes Phase-Field Method (NS-PFM)**

The NS-PFM used in this study has been proposed for immiscible, incompressible, isothermal two-phase flows with high density ratio (Takada et al 2005, 2006a-d), based on two-phase LBM (Chen & Doolen 1998, Inamuro et al 2004, Takada et al 2001, Succi 2001). It solves a set of the following mass and momentum conservation equations, and the Cahn-Hilliard (CH) equation governing time evolution of the diffusive interfacial profile (Anderson et al 1998, Badalassi et al 2003, Swift et al 1996),

\[
\nabla \cdot \mathbf{u} = 0, \\
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla \cdot (\mathbf{P} + \nabla \phi), \\
\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u} - \Gamma \nabla \eta) = 0.
\]

In the CH equation (3), the continuous scalar variable $\phi$ is an index function (so-called order parameter) to describe the diffusive interface profile (Anderson 1998, Badalassi 2003). In this study, the chemical potential $\eta$ is derived from a free-energy functional $\Psi_f$ with the van-der-Waals bulk energy $\psi(\phi)$ (Inamuro et al 2004, Seta et al 2004&2006, Teng et al 2000) and an excessive energy caused by the local gradient of $\phi$,

\[
\eta = \frac{\delta \Psi}{\delta \phi} = \frac{\partial \psi}{\partial \phi} - \kappa_d \nabla^2 \phi
\]

where $\psi$ takes the double-well form on $\phi$, $\kappa_d$ is one of parameters to control interfacial thickness. For simplicity of computation, the mobility $\Gamma$ on $\phi$ in Eq.(3) is defined as,

\[
\Gamma = \Gamma_0 \phi,
\]

where the factor $\Gamma_0$ is set to be a positive constant.

Inside the interface, the density $\rho$ is defined as a sine-curve function of $\phi$ (Inamuro et al 2004) and varies between given constants $\rho_0$ and $\rho_1$ of gas and liquid phases,

\[
\rho = \frac{\rho_1 + \rho_0}{2} + \frac{\rho_1 - \rho_0}{2} \sin \left( \frac{\phi - \phi_k}{\phi_l - \phi_k} \pi \right).
\]

where $\phi_l$ and $\phi_k$ are arbitrary thresholds for the index $\phi$ to distinguish the phases. The viscosity $\mu$ in the Newtonian stress tensor $\tau$ also varies between given constants $\mu_0$ and $\mu_1$, as a function of $\rho$ (Inamuro et al 2004),

\[
\mu = \mu_0 + \frac{\mu_1 - \mu_0}{\rho_1 - \rho_0} (\rho - \rho_0).
\]

The pressure tensor in Eq.(2), $\mathbf{P}$, is expressed as follows (Anderson 1998, Nadiga & Zaleski 1996),

\[
\mathbf{P} = \left( p - \kappa_S \rho \nabla^2 \rho - \frac{\kappa_d}{2} |\nabla \rho|^2 \right) \mathbf{I} + \kappa_d \nabla \rho \otimes \nabla \rho
\]

$p$ is the pressure in homogeneous field. The parameter $\kappa_S$ constant in the whole flow field is determined from the definition of surface tension $\sigma$ as an excessive free energy per unit area on a flat interface (Cahn & Hilliard 1958),

\[
\sigma = \kappa_S \int_{-\infty}^{\infty} \left( \frac{\partial \rho}{\partial \xi} \right)^2 d\xi,
\]
where the direction of $\xi$ is normal to the interface. By substituting Eq.(10) into Eq.(2) and doing some algebraic operation, the pressure term is reduced into the following simple form of two gradient terms.

$$\nabla \cdot \mathbf{P} = \nabla p - \rho \kappa_{i} \nabla^{2} \rho$$  \hspace{1cm} (12)

**Initial Setting of Interface in NS-PFM Simulation**

**Pre-evaluation of surface tension**

As described in Eq.(11), the surface tension $\sigma$ in the phase-field method is equivalent to the free-energy increase induced by the density gradient. In this study, the value of $\sigma$ is determined as follows (Takada et al. 2006a-d).

(1) Maximum and minimum values of the index function $\phi_{\max}$ and $\phi_{\min}$ are calculated using a given set of parameters, $A$, $B$, and $T$, in Eq. (6) according to the Maxwell rule (Seta et al. 2004&2006).

(2) $\phi(\xi)$ across a flat interface is computed under the equilibrium condition at a given value of $\kappa_{i}$:

$$\eta(\phi) = \text{constant} \quad \left( \eta(\phi_{\max}) = \eta(\phi_{\min}) \right)$$  \hspace{1cm} (13)

(3) The density distribution $\rho(\xi)$ is computed by substituting $\phi(\xi)$ into Eq. (8).

(4) The density gradient is calculated using a fourth-order central difference scheme.

(5) Equation (11) is integrated numerically using Simpson’s rule.

(6) The value of $\kappa_{i}$ is determined as $\sigma / (\text{integral value of Eq. (11)})$.

**Figure 1:** Profiles of index function $\phi$ and density $\rho$ across a flat interface with normal axis $\xi$.

**Table 1:** Profile of index function $\phi$ across a flat interface for $A=B=1$ and $T=0.293$

<table>
<thead>
<tr>
<th>$\kappa_{i}$</th>
<th>Max</th>
<th>$\phi/d \xi$</th>
<th>Integral $(d \phi/d \xi)^2$</th>
<th>Thickness $l_{\phi}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.005499</td>
<td>0.006941</td>
<td>2.833</td>
<td></td>
</tr>
<tr>
<td>0.02</td>
<td>0.002750</td>
<td>0.004908</td>
<td>4.006</td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>0.001100</td>
<td>0.003104</td>
<td>6.335</td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>0.000550</td>
<td>0.002195</td>
<td>8.959</td>
<td></td>
</tr>
</tbody>
</table>

**Table 2:** Profile of fluid density $\rho$ across a flat interface for $A=B=1$ and $T=0.293$

<table>
<thead>
<tr>
<th>$\kappa_{i}$</th>
<th>Max</th>
<th>$\rho/d \xi$</th>
<th>$\sigma/\kappa_{i}$</th>
<th>Thickness $l_{\rho}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.001101</td>
<td>7.972E-07</td>
<td>1.251</td>
<td></td>
</tr>
<tr>
<td>0.02</td>
<td>0.000778</td>
<td>5.637E-07</td>
<td>1.770</td>
<td></td>
</tr>
<tr>
<td>0.05</td>
<td>0.000492</td>
<td>3.565E-07</td>
<td>2.798</td>
<td></td>
</tr>
<tr>
<td>0.10</td>
<td>0.000348</td>
<td>2.521E-07</td>
<td>3.957</td>
<td></td>
</tr>
</tbody>
</table>

Figure 1 shows the spatial distributions of $\phi(\xi)$ and $\rho(\xi)$ across a flat interface with normal vector in the $\xi$ direction, which are theoretical solutions in an equilibrium state under the condition of $A=B=1$, $T=0.293$, $\kappa_{i}=0.1$, $\phi_{\text{min}}=0.2751$, and $\phi_{\text{max}}=0.3802$. The continuous variation region of $\rho(\xi)$ from $\rho_{\text{L}}$ to $\rho_{\text{G}}$ is narrower than that of $\phi(\xi)$ due to Eq.(8) with the thresholds $\phi_{\text{min}}$ and $\phi_{\text{max}}$.

The widths on $\phi$ and $\rho$, interfacial thickness $l_{\phi}$ and $l_{\rho}$, are represented by the following linear approximations.

$$l_{\phi} = \left( \phi_{\text{max}} - \phi_{\text{min}} \right) \left( \int_{-\infty}^{+\infty} \left( \frac{\partial \phi}{\partial \xi} \right)^2 d\xi \right)^{-1}$$  \hspace{1cm} (14)

$$l_{\rho} = \left( \rho_{\text{L}} - \rho_{\text{G}} \right) \left( \int_{-\infty}^{+\infty} \left( \frac{\partial \rho}{\partial \xi} \right)^2 d\xi \right)^{-1}$$  \hspace{1cm} (15)

As shown in Fig. 2, in addition to Tables 1 and 2, they are proportional to $\kappa_{i}^{2.5}$, respectively.

![Figure 2: Interfacial thickness $l_{\phi}$ and $l_{\rho}$ of the index function $\phi$ and the density $\rho$.](image)

**Initialization of spatial two-phase distribution**

In advance of the simulation of two-phase fluid motions, the index function $\phi$ in the whole flow field is initialized using only the CH equation (3), which is numerically solved to obtain the steady-state solution of $\phi$ under the equilibrium condition at $u=0$. The initial values of $\phi$ inside liquid and gas phases on of a curved interface were set to be smaller than $\phi_{\text{min}}$ and $\phi_{\text{max}}$ for flat interface, respectively. This operation makes it possible to balance the chemical potential $\eta$ more exactly over the whole flow field (Takada et al. 2006b), thus preventing the generation of local diffusive current of $\phi$ dependent on interfacial curvature (Gibbs–Thomson effect (Jacqmin 1999)).

**Boundary Condition on Wetting Solid Surface**
In the same way as other phase-field methods (Brian et al 2002, Seppecher 1996, Yoshino & Mizutani 2006), a wetting boundary condition on surface of solid wall is incorporated into the NS-PFM through the following equation (Takada & Tomiyama 2007),

\[ n \cdot \kappa_s \nabla \phi = -\gamma_s, \quad (16) \]

where \( n \) is the unit vector normal to the solid boundary and the parameter \( \gamma_s \) is called as wetting potential. The above equation is derived from a free-energy functional \( \Psi \) of the whole fluid system including the solid boundary,

\[ \Psi_{\text{system}} = \Psi_{\phi} - \int_S \gamma_s \phi dS, \quad (17) \]

where \( \gamma_s \) denotes the free-energy increase per unit area of the solid surface (Jamet 2001, Briant 2002). The contact angle \( \theta_v \) of liquid phase on the surface depends on the local value of \( \gamma_s \). In addition to Eq.(16), the following constraints are also imposed on the stationary solid surface as a non-slip and no-flux boundary:

\[ \begin{align*}
  n \cdot \nabla p &= 0 \quad (18) \\
  n \cdot \nabla \eta &= 0 \quad (19) \\
  u &= 0 \quad (20)
\end{align*} \]

**Numerical Scheme**

In this study, a set of Eqs. (1)-(3) is numerically solved using conventional simple Eulerian-approach techniques mentioned below (Takada et al 2005 & 2006a-d). The three-dimensional space is discretized uniformly using cubic cells with width \( \Delta x=\Delta y=\Delta z=1 \) on a fixed grid in Cartesian coordinate system (x, y, z), where scalar and vector variables are located in staggered arrangement respectively. The scalar variables on cell surfaces are interpolated with a fourth-order scheme. Time marching to update \( u \) and \( \phi \) in Eqs.(2) and (3) is based on the second-order Runge-Kutta's scheme with a constant increase \( \Delta t \). At each time step, the solenoidal velocity \( u \) satisfying Eq.(1) and the scalar variable of pressure \( p \) are calculated using the projection algorithm (Chorin 1968), where successive over-relaxation method is used for solving the Poisson equation on \( p \),

\[ \nabla \cdot \left( \frac{1}{\rho} \nabla p \right) = \nabla \cdot \frac{u'}{\Delta t}. \quad (21) \]

The provisional velocity \( u' \) is explicitly calculated from the known data at each time step using the equation of motion without the pressure term. Finally, the solenoidal \( u \) at next time step which satisfies Eq.(1) is obtained from \( p \) and \( u' \) by using the following correction (Chorin 1968).

\[ u = u' - \frac{\Delta t}{\rho} \nabla p \quad (22) \]

The advection term in Eq.(2) was calculated with a third-order upwind finite difference scheme (Kawamura & Kuwahara 1986), while that in the CH equation (3) was calculated with a fourth-order central difference scheme (CDS) mentioned below. Gradients of the scalar variables \( (\phi, \rho, \text{and } p) \) were evaluated with a forth-order CDS, while a second-order CDS was applied to the viscous term.

The conservation of \( \phi \) in the whole computational domain was ensured by setting a central finite difference of the advection term of Eq.(3) according to a finite volume scheme given by

\[ \frac{\partial F_{\phi}}{\partial x} \approx \frac{F_{\phi,i+1/2} - F_{\phi,i-1/2}}{\Delta x}, \quad (23) \]

\[ F_{\phi,i+1/2} = -F_{\phi,i+1} + 26F_{\phi,i} - F_{\phi,i-1}, \quad (24) \]

where the subscript \( i \) denotes the cell number in the \( x \) direction, and \( F_{\phi,i+1/2} \) on a cell surface of the \( i \)th cell represents the summation of \( x \)-direction volume fluxes of \( \phi \) due to the flow velocity \( u \) and the current \( -\nabla \eta \) in Eq.(3). The scalar variable \( \phi \) on the cell surface \( i+1/2 \) is calculated by interpolating the values at four neighboring cells as follows:

\[ \phi_{i+1/2} = \frac{1}{16} \left[ \phi(\phi_{(i+1)} + \phi_{(i+2)}) - \phi_{(i+2)} - \phi_{(i+1)} \right]. \quad (25) \]

As for the calculation of the third-order differential term on the right-hand side of Eq. (3), the following fourth-order central difference scheme is applied to the first-order differential term on \( \nabla^2 \phi \) in the same way as the other scalar variables:

\[ \frac{\partial \nabla^2 \phi}{\partial x} \bigg|_{i+1/2} \approx \frac{\nabla^2 \phi_{i+2} + 27 \left( \nabla^2 \phi_{i+3} + \nabla^2 \phi_{i} \right) + \nabla^2 \phi_{i}}{24\Delta x}. \quad (26) \]

\[ \nabla^2 \phi \] is computed using a fourth-order CDS.

**Numerical Results and Discussion**

This section describes numerical results of two-phase flows obtained with the above-mentioned NS-PFM. All the simulations have been carried out on the fixed spatial grid with uniform mesh of \( \Delta x=\Delta y=\Delta z=1 \) in 3D. In the flow field, a surface of solid wall was treated as a no mass flux and non-slip boundary. In the simulations under no gravity, the contact angle \( \theta_v \) of liquid phase on the surface depends on the local value of \( \gamma_s \). In addition to Eq.(16), the following constraints are also imposed on the stationary solid surface as a non-slip and no-flux boundary:

\[ \begin{align*}
  n \cdot \nabla p &= 0 \quad (18) \\
  n \cdot \nabla \eta &= 0 \quad (19) \\
  u &= 0 \quad (20)
\end{align*} \]

**Static contact angle**

In order to examine the validity of the NS-PFM plus the wetting boundary condition, Eq.(16), we first conducted numerical simulation of formation of three-dimensional single drop in a stagnant gas on a flat surface of stationary solid wall. In this case, the surface tension \( \sigma=7.42 \times 10^{-3} \) was given by \( \kappa_s=2.94 \times 10^{-2} \). The densities \( \rho_s \) and \( \rho_g \) were given by \( \rho_s=1.247 \times 10^3 \) and \( \rho_g=1.0 \) respectively, while both the viscosities \( \mu_s \) and \( \mu_g \) were set to be 0.01. The drop initially took a hemispherical shape with radius of about 15\( \Delta x \). Figures 3 and 4 show the numerical results of steady-state interfacial shape of the drop and cross-sectional distributions of \( \phi \) and \( \rho \). The interface with thickness of about 4\( \Delta x \) in the \( \rho \) field
is represented by a contour surface with the medium value \((\rho_c + \rho_L)/2\). As shown in Fig.5, the measured value of \(\theta_W\) varied almost linearly from 49° to 134° for the given value of \(\gamma_S\) between \(\pm 1.5 \times 10^{-3}\) (Takada & Tomiyama 2007).

**Figure 3:** The interfacial shape and the static contact angle \(\theta_W\) of the liquid drop on a flat solid surface in a stagnant gas under no gravity for \(A=B=1\), \(T=0.293\), \(\kappa_g=0.1\) and wetting potential \(\gamma_S=10^{-3}\) to \(10^{-3}\).

**Figure 4:** The spatial distributions of \(\phi\) and \(\rho\) on a cross section of the liquid drop with static contact angle \(\theta_W\) on a flat solid surface in a stagnant gas under no gravity, for \(A=B=1\), \(T=0.293\), \(\kappa_g=0.1\) and wetting potential \(\gamma_S=10^{-3}\) to \(-10^{-3}\).

**Figure 5:** The static contact angle \(\theta_W\) of the liquid drop on a flat solid surface in a stagnant gas under no gravity, for \(A=B=1\), \(T=0.293\), \(\kappa_g=0.1\) and wetting potential \(\gamma_S=-1.75 \times 10^{-3}\) to \(1.5 \times 10^{-3}\).
Two-phase fluid motion in micro channel

The NS-PFM was then applied to numerical simulations of motion of incompressible isothermal two-phase fluid in a rectilinear micro channel with a y-z cross section of sides \( L_y = L_z = 20 \) (Takada & Tomiyama 2007). The fluid had the same density and viscosity ratios \( \rho_L/\rho_G = 828 \) and \( \mu_L/\mu_G = 55 \) as those of an air-water system, while the effect of surface tension \( \sigma = 5.95 \times 10^{-3} \) or \( 5.95 \times 10^{-1} \) in the simulations was equivalent to \( 10^{-3} \) or \( 10^{-3} \) times smaller than that of the actual system, for the sake of numerical stability at \( \Delta t = 2.5 \times 10^{-3} \) or \( 5 \times 10^{-3} \). As shown in Fig.6, the three-dimensional computational domain was surrounded by hydrophobic flat solid walls with \( \gamma_L = 1.044 \times 10^{-3} \), liquid inflow boundary, and free outflow boundary under constant pressure. The liquid phase with \( \rho_L = 1 \) was injected into the channel under the inflow condition of either (A) uniform constant velocity \( \mathbf{u}_i \) or (B) constant pressure gradient \( \partial p/\partial \mathbf{x} \). On the bottom wall surface, a hydrophilic region with width \( \alpha \) and the wetting potential \( \gamma_L = -1.044 \times 10^{-2} \) was placed away from the initial position of the interface. The static contact angles \( \theta_w \) on the hydrophilic and hydrophobic surfaces were about 61° and 119°, respectively.

Figure 6: Schematic of the computational domain in the simulation of two-phase fluid in a rectilinear channel for density and viscosity ratios \( \rho_L/\rho_G = 828 \) and \( \mu_L/\mu_G = 55 \).

Figure 7: Side-view snapshots of the two-phase fluid moving in the rectilinear channel with height \( L_z = 20 \Delta z \) at dimensionless time \( t' = t|U_{inflow}/L_y| = 3.60 \times 10^{-2} \) for \( \text{Ca}=\mu_L|U_{inflow}|/\sigma = 0.275 \) and \( \text{Re}=\rho_L L_y|U_{inflow}|/\mu_L = 1.99 \times 10^{-2} \) under the uniform inflow boundary condition (A) of \( |U_{inflow}|=1.28 \times 10^{-3} \). The lower leading edge of the liquid on the bottom wall moved faster than the upper one in each case, because the former one was accelerated by the capillary force of the hydrophilic surface. The lower leading edge also moved faster as the hydrophobic region was more widened. In contrast, the upper edge moved more slowly as increasing \( \alpha \). This is because of the incompressibility of the fluid and the inflow condition of the constant velocity \( \mathbf{u}_i \).

Figure 8a: Side-view snapshots of the velocity distribution of the two-phase flow on x-z central cross section of the rectilinear channel with height \( L_z = 20 \) at \( t' = |U_{inflow}/L_y| \) for \( \text{Ca}=\mu_L|U_{inflow}|/\sigma = (a) 0.77 \) and (b) \( 7.7 \times 10^{-1} \). The red-colored bold solid line denotes the hydrophilic region of the wall surface with \( \theta_w = 61^\circ \).
The numerical results under the inflow condition (B) of constant $\partial p/\partial x=-3.276\times10^{-3}$ are shown in Fig. 8. On the hydrophilic region, the lower leading edge of the liquid for (a) $Ca=0.77$ moved more slowly than that for (b) smaller $Ca=7.7\times10^{-3}$ ($10^2$ times larger $\sigma$). In the latter case, local counter-clockwise circulation flow was caused around the interface by the capillary force pulling the liquid phase just after the lower leading edge started moving on the hydrophilic region, as shown in Fig. 8a (3) at dimensionless time $t^*=0.108$. In contrast, the circulation flow was not induced in the former case of larger $Ca$, because the inertia force due to the pressure gradient at the inflow boundary was dominant over the surface tension force. The fluid motion at smaller $Ca$ was accelerated in the whole flow domain by the local effect of the surface tension and the hydrophilic capillarity on the fluid interface more than that at larger $Ca$, as shown in Fig. 9 ($|U_{in avg}|$ is the average magnitude of the inflow velocity on the cross section with area $L_x\times L_z$ at $x=0$). The result of the acceleration of two-phase flow in this simulation agreed qualitatively with experimental data of gas-liquid flows in micro-channels.

\[ C_a = \mu_\ell |U_{in avg}|/\sigma \]

\[ |U_{in avg}| = 3.60 \times 10^{-3} \]

\[ L_x = 20 \]

\[ \mu_\ell = 1.282 \]

Figure 8b: Side-view snapshots of the velocity distribution of the two-phase flow on $x$-$z$ central cross section of the rectilinear channel with $L_z=20$ at $t^*=t|U_{in avg}|/L_z$, for $Re=0.56$, $Ca= (a) 0.77$ and (b) $7.70\times10^{-3}$. The red-colored bold line denotes the hydrophilic wall surface of $\theta_w = 61^\circ$.

\[ x=0.5 \]

\[ C_a = \mu_\ell |U_{in avg}|/\sigma \]

\[ |U_{in avg}| = 3.60 \times 10^{-3} \]

\[ L_x = 20 \]

\[ \mu_\ell = 1.282 \]

Figure 9: Time series of the velocity component $u(x)$ in $x$ direction at $x=0.5\Delta x$ and $25.5\Delta x$ ($\Delta x=1$) along the center line of the channel for $Re=\rho_L|U_{in avg}|/\mu_\ell=0.56$.

Motions of single drop on solid surface with heterogeneous wettability

The third application of the NS-PFM with the wetting boundary condition was a series of displacement and breakup motions of single liquid drop sustained on a flat solid surface in a stagnant gas under no gravity in three dimensions. The simulation has been conducted for evaluating the fundamental capability of the NS-PFM to predict drop motions in micro-fluidics devices using EWOD technology (Berthier et al 2006).

The computational domain was discretized with $64\times64\times32$ cubic mesh units and surrounded with stationary flat solid walls. The drop of $\rho_D=1$ and $\mu_D=1.67\times10^3$ was initially placed on the bottom solid wall to be formed of a hemisphere with radius $R=16\Delta y$ in the gas of $\rho_G=1$ and $\mu_G=2.26\times10^5$. The motions of the drop were simulated under several conditions of difference between contact

\[ \rho_D=1 \]

\[ \mu_D=1.67\times10^3 \]

\[ \rho_G=1 \]

\[ \mu_G=2.26\times10^5 \]
angles on hydrophilic and hydrophobic regions of the solid surface, \( \Delta \theta_{h_2} = \theta_{h_1} - \theta_{h_2} > 0 \), and Ohnesorge number \( Oh \),

\[
Oh = \frac{\mu_s}{\sqrt{\rho_s R \sigma}}.
\]  

(27)

In the simulation of displacement motion, as shown in Fig.10, the center of bottom face of the drop was initially positioned just on the border line between the hydrophilic and hydrophobic surfaces of the wall. The contact angle difference \( \Delta \theta_h \) was set to be either 58°, 68°, or 86° by using \( \gamma_h = \pm 1.044 \times 10^{-3}, \pm 1.25 \times 10^{-3} \) or \( \pm 1.50 \times 10^{-3} \). The values of \( Oh \) were \( 1.2 \times 10^{-3}, 1.7 \times 10^{-3} \) and \( 2.4 \times 10^{-3} \), for \( \sigma = 6.06 \times 10^{-2}, 3.03 \times 10^{-2} \) and \( 1.21 \times 10^{-2} \), respectively (see Table 3).

![Figure 10: Schematic of the computational domain for the numerical simulation of liquid drop displacement on a flat solid surface in a gas under no gravity \( g = 0 \).](image)

**Table 3:** The values of wetting potential \( \gamma_h \), contact angle difference \( \Delta \theta_h = \theta_{h_1} - \theta_{h_2} \) on the solid surface and Ohnesorge number \( Oh = \mu_s / (\rho_s \sigma R)^{0.5} \) in the drop displacement simulation \( (\mu_s = 1.67 \times 10^{-3}, \rho_s = 1 \) and \( R = 16 \))

<table>
<thead>
<tr>
<th>Case No.</th>
<th>( \gamma_h )</th>
<th>( \Delta \theta_h ) (degree)</th>
<th>( Oh ) ( (\times 10^{-8}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \pm 1.044 \times 10^{-3} )</td>
<td>58</td>
<td>1.70</td>
</tr>
<tr>
<td>2</td>
<td>( \pm 1.25 \times 10^{-3} )</td>
<td>68</td>
<td>86</td>
</tr>
<tr>
<td>3</td>
<td>( \pm 1.50 \times 10^{-3} )</td>
<td>86</td>
<td>86</td>
</tr>
<tr>
<td>4</td>
<td>( \pm 1.044 \times 10^{-3} )</td>
<td>58</td>
<td>2.40</td>
</tr>
<tr>
<td>5</td>
<td>( \pm 1.25 \times 10^{-3} )</td>
<td>86</td>
<td>1.20</td>
</tr>
</tbody>
</table>

Figure 11 shows the result of the drop shape and the velocity distribution for Case1 at \( Oh = 1.7 \times 10^{-3} \), in which the gas and the liquid were assumed to be air and water at 1 atm and at room temperature, respectively. The drop moved onto the hydrophilic region out of the hydrophobic region due to the capillary force difference. The displacement was caused in all the cases. As shown in Fig.12a, the drop motion was more accelerated as increasing \( \Delta \theta_h \) and as decreasing \( Oh \) (for larger \( \sigma \)). For different \( Oh \) at \( \Delta \theta_h = 58° \), however, the moving distance of center of mass of the drop did not change under dimensionless time \( t^* = (\sigma \rho_s^{-1} R^{1/2}) \) (see Fig.12b).

In the drop breakup simulation, the hydrophobic region with width \( a \) was set on the central part of the bottom wall, while the hydrophilic regions with width \( 32\Delta y \times 2 \) were located on the both sides. In the same way as the displacement simulation, a hemispherical liquid drop with radius \( R \) was initially placed on the central part of the bottom wall surface (Fig.13).

![Figure 12a: The moving distance of center of mass of the liquid drop at time \( t \).](image)

![Figure 11: Snapshots of the drop shape and the velocity distribution on a y-z vertical cross section at time \( t^* = t \) \( (\sigma \rho_s^{-1} R^{1/2}) \) in Case1 (see Table 3).](image)
The breakup simulation was carried out under the conditions of \( \Delta \theta_W = 29^\circ, 58^\circ, 68^\circ, 86^\circ \), \( a^* = a/R = 0.5, 1.0, 1.5 \), and \( Oh = 1.2 \times 10^{-3} \) to \( 3.39 \times 10^{-3} \). As shown in Table 4, the drop did not break up in Case9 and Case10 for \( \Delta \theta_W = 29^\circ \), and in Case12 for \( a^* = 0.5 \). In the other cases, the drop broke up into smaller daughters, as shown in Figs.14 and 15. In all the cases of breakup, the center of mass of half part of the drop moved from its initial position over dimensionless distance 0.4. Time series of the moving distance at \( t' \) did not change for different \( Oh \) at \( \Delta \theta_W = 58^\circ \) (see Fig.16).
In this study, a computational fluid dynamics phase-field method, NS-PFM (Takada et al 2005 & 2006a-d), was applied to several problems of motion of incompressible isothermal two-phase fluid with high density ratio on solid surface with heterogeneous wettability, for examining the fundamental capability to simulate the motions in various micro-fluidics devices. NS-PFM combines Navier-Stokes equations with the phase-field model for multiphase interface based on the van der Waals-Cahn-Hilliard free-energy theory. A simple wetting boundary condition on the solid surface was proposed for the flow with high density ratio and incorporated into the method through the same free-energy-based approach as other phase-field methods, where a free-energy increase per unit area of the solid surface in the fluid was assumed to be proportional to a parameter of wetting potential of the surface.

The following major findings were obtained through the NS-PFM simulation of the two-phase flows with density ratio about 800 under no gravity in three dimensions: (1) The static contact angle of liquid drop on solid surface varies almost linearly with the value of the wetting potential parameter. (2) The interfacial motion of the two-phase fluid in a rectilinear channel is accelerated on hydrophilic region of the solid surface. (3) The motion of the fluid in the channel is accelerated in the whole flow domain for larger surface tension. This numerical result agrees qualitatively with experimental data in air-water system. (4) NS-PFM successfully captures displacement

**Conclusions**
and breakup motions of single liquid drop on a flat solid wall caused by difference between the capillary forces on the hydrophilic and hydrophobic regions. (5) The motions of the drop on the wall depend on surface tension of the fluid interface, contact angles and widths of hydrophilic and hydrophobic regions of the surface.

The above-mentioned numerical results give the sufficient proof that NS-PFM with the proposed wetting boundary condition has a potential to simulate capillarity-driven two-phase flows with high density ratio equivalent to that of air-water system. The applicability of the method to micro-fluidics simulations, however, has been still examined more qualitatively and quantitatively in comparison with other numerical and experimental data. One of the future works is to reduce the parasitic currents around the interface for smaller capillary or Ohnesorge number by adopting the energy-conserved spatial discretization scheme (Jamet et al 2002) to solve the NS and CH equations for the microscopic two-phase flows, where the surface tension force becomes dominant over the inertia and viscous forces. After more works, NS-PFM will be finally applicable to the simulations of micro fluids in bio-chemical \( \mu \)-TAS, electronic paper and energy-efficient display, which can control the motions of the fluid particles at high frequency using EWOD technology (Berthier et al 2006, Feenstra et al 2006, Northrup et al 2003).

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