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NUMERICAL SIMULATION OF TWO-PHASE FLUID MOTION IN MICROCHANNEL BASED ON PHASE-FIELD MODEL

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Abstract. Allen-Cahn (AC) and Cahn-Hilliard (CH)-type diffuse-interface advection equations based on a phase-field model (PFM) are evaluated for computational fluid dynamics (CFD) simulation of motions of microscopic immiscible incompressible isothermal two-phase fluid contacting solid surface. For solving a conservation-modified AC equation, a lattice-Boltzmann method (LBM) based on fictitious mesocsopic particle kinematics is adopted. The modified AC and CH equations without interfacial curvature-induced diffusion flux are tested through a benchmark problem of interfacial advection. It is confirmed that both the volume and the shape of fluid with diffusive interface are well conserved during the advection. In addition, for developing a novel micro-fabrication process of flexible and large-area sheet display device, immiscible liquid-liquid two-phase slug droplets formation in T-junction microchannel with square cross section and hydrophilic solid walls is investigated through CFD simulation using a PFM-based method. It adopts the semi-Lagrangian LBM scheme to second-order accuracy in both space and time for solving the modified AC equation with Navier-Stokes equations. The ratio of volumetric flow rate of dispersed phase to that of continuous phase is fixed at 1.0 within low capillary, Reynolds and Weber numbers for silicone oil-pure water system with hydraulic diameter of 100 μm, kinematic viscosity of 1.0 cSt. and interfacial tension of 41.6 mN/m. The major findings are as follows: (1) the PFM-CFD method predicts well pressure increase inside spherical droplet proportional to interfacial curvature in agreement with the Laplace-law solution; (2) the continuous-phase (water) and dispersed-phase (oil) slug droplets become shorter at nearly-constant length difference between them as their flow rates are increased; (3) the length and volume fraction of the droplet in the simulation agree well with experimental data.

1 INTRODUCTION

Microscopic gas-liquid and liquid-liquid flows with a fluid-fluid interface on a heterogeneously or homogeneously wettable solid surface are widely encountered in various science and engineering fields. It is often difficult to experimentally observe such flows and measure the velocity and the pressure simultaneously in three dimensions or to analyse

theoretically them by the classical continuum dynamics approach based on a sharp-interface model. Computational fluid dynamics (CFD) simulations facilitate the understanding and prediction of the two-phase flows for flexible and accurate control of fluid-particle motion and position; as its result, micro-fluidic devices and micro-electro-mechanical-systems (MEMS) device fabrication processes can be optimally designed [1,2].

In this study, we have examined the applicability of two types of diffuse-interface advection equation based on a phase-field model (PFM) [3] to the simulation of two-phase fluid motion on solid surface. PFM has recently been attracting much attention from many researchers as one of mesoscopic models which efficiently simulate behaviour of multi-phase system. Based on the free-energy theory, PFM describes an interface as a finite volumetric zone between different phases, across which physical properties vary steeply but continuously. Two-phase coexistence is allowed by a free-energy functional which has a double-well potential of an order parameter and its squared local gradient term, without imposing topological constraints on interface as phase boundary. The contact angle, depending on the energy balance among three types of interfaces, is obtained from a potential of the solid surface through a simple boundary condition of the gradient of the order parameter on the surface. As a result, the PFM-based CFD method does not necessarily require conventional elaborating algorithms for advection and reconstruction of interfaces [4-7]. The method therefore has an advantage over other methods of easy calculation of multiple-interface advection with deformation on a partially-wettable solid surface.

This paper is organized as follows. In the next section, we outline a PFM-based CFD method that we have proposed for simulation of immiscible liquid-liquid two-phase flow [8, 9]. The method adopts a conservation-modified diffuse-interface advection equation [7] and a numerical solution scheme based on a lattice-Boltzmann method (LBM) [10, 11]. In the third section, we present benchmark test results on two-dimensional linear translation of a circular-shaped interface by use of two kinds of PFM-based advection equation [8] and the CFD simulation result of a mono-dispersed two-phase slug flow in a micro channel with a T-shaped junction [9, 12, 13]. The conclusions are described in the last section.

2 BASIC EQUATIONS IN PHASE-FIELD MODEL (PFM)

The PFM-based methods for simulating incompressible isothermal viscous two-phase fluid flows adopt the following set of mass and momentum conservation equations with an interface advection equation [3-9, 11]:

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

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \frac{1}{\rho}\left(-\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{F}_I\right) \tag{2}$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \left(\phi \mathbf{u} - D(\phi)\nabla \phi\right) = 0 \tag{3}$$

where $\mathbf{u}$ denotes the velocity; t, the time; ρ, the density; p, the pressure; $\boldsymbol{\tau}$, the viscous stress tensor; $\mathbf{F}_I$, the interfacial-tension force; ϕ, the order parameter which indicates each phase and interfacial regions with its continuous values; and $D(\phi)$, the diffusivity. In well-known Cahn-Hilliard (CH) form [3-6, 11], the diffusion term of Eq. (3) includes the following coefficient:

$$D(\phi) = M_{CH} \frac{\partial \eta(\phi)}{\partial \phi} \tag{4}$$

$$\eta(\phi) = \frac{\partial \psi_0}{\partial \phi} - \kappa_\phi \nabla^2 \phi \tag{5}$$

where M_{CH} denotes the mobility; η, the chemical potential; ψ_0, the double-well potential on ϕ ; and κ_ϕ, the capillary coefficient which is related with interfacial width and tension. In contrast to the CH form, a conservation-modified Allen-Cahn (AC) form [7] adopts the following diffusion coefficient in Eq. (3):

$$D(\phi) = M_{AC} \kappa_\phi \left(1 - \frac{\partial \phi(\xi)}{\partial \xi} \left| \nabla \phi \right|^{-1} \right) \tag{6}$$

$$\phi(\xi) = \frac{1}{2} \left\{ 1 + \tanh \left(\frac{\xi}{2\sqrt{\kappa_\phi}} \right) \right\} \tag{7}$$

where M_{AC} denotes the mobility; and ξ, the signed distance in the direction normal to the interface from the central position at $\xi = 0$. The profile of ϕ across a flat interface in an equilibrium state is theoretically expressed by use of Eq. (7).

In each of the CH and AC forms, the diffusion term of Eq. (3) disappears in an equilibrium state. The AC equation, Eq. (3) plus Eq. (6), is equivalent to a conservative level-set equation [12] in one-step form by which both of interfacial re-initialization and advection calculation are done at the same moment [7]. The idea for removing the interfacial-curvature dependency on diffusion of ϕ from the original AC equation is also applicable to the coefficient Eq. (4) for the CH equation [8].

3 NUMERICAL METHOD FOR TWO-PHASE FLOW

For solving the above-mentioned set of Eqs. (1), (2) and (3) with Eqs. (6) and (7), we have proposed a numerical scheme [8, 9] based on lattice Boltzmann method (LBM) [10, 11]. LBM assumes that a macroscopic fluid consists of fictitious mesoscopic particles repeating collisions with each other and linear translations with a set of isotropic discrete velocities. The main variables in LBM are distribution functions of number density of the particles grouped with their velocities. Time evolutions of the distribution functions, f_a and g_a, at position $\mathbf{x}$ and at time t are expressed by

$$\frac{\partial f_a}{\partial t} + \mathbf{e}_a \cdot \nabla f_a + \frac{\mathbf{F}_I}{\rho} \cdot \frac{\partial f_a}{\partial \mathbf{e}_a} = -\frac{1}{\tau_f} \left[f_a(\mathbf{x},t) - f_a^{eq}(\mathbf{x},t) \right] \tag{8}$$

$$\frac{\partial g_a}{\partial t} + \mathbf{e}_a \cdot \nabla g_a = -\frac{1}{\tau_g} \left[g_a(\mathbf{x},t) - g_a^{eq}(\mathbf{x},t) \right] \tag{9}$$

where $\mathbf{e}_a$ is the particle velocity vector; the subscript a, index of the velocity set; τ_f and τ_g , the relaxation times for f_a and g_a respectively in the BGK approximation collision operator; and the superscript eq denotes a local equilibrium state.

In this study, Equations (8) and (9) are discretized respectively into the semi-Lagrangian forms with second-order accuracies in both space and time as follows [8, 9]:

$$f_a\left(\mathbf{x},t'\right)=f_a\left(\mathbf{x}-\mathbf{e}_a\Delta t,t\right)-\frac{\Delta t}{\tau_f}\left[f_a\left(\mathbf{x}-\mathbf{e}_a\Delta t,t\right)-f_a^{eq}\left(\mathbf{x}-\mathbf{e}_a\Delta t,t\right)\right] \tag{10}$$

$$f_a\left(\mathbf{x},t+\Delta t\right)=f_a\left(\mathbf{x},t'\right)+3w_a\Delta t\frac{\mathbf{e}_a\cdot\mathbf{F}_I}{c^2} \tag{11}$$

$$g_a\left(\mathbf{x}+\mathbf{e}_a\Delta t,t+\Delta t\right)=g_a\left(\mathbf{x},t\right)-\frac{\Delta t}{\tau_g}\left[g_a\left(\mathbf{x},t\right)-g_a^{eq}\left(\mathbf{x},t\right)\right] \tag{12}$$

where Δt is the constant increase in time, $\mathbf{x}+\mathbf{e}_a\Delta t$ denotes the position neighboring $\mathbf{x}$ in the direction of the vector $\mathbf{e}_a$, and w_a is the weight parameter. In three-dimensional Cartesian coordinate system (x, y, z), the space is divided uniformly into unit cubic cells with sides:

$$\Delta x=\Delta y=\Delta z=c\Delta t \tag{13}$$

where c is the lattice constant. The particles are set to be rest or to move according to three-dimensional 15-velocity model [10, 11]. The scalar and vector variables of two-phase fluid, ρ, $\mathbf{u}$, p and ϕ, are co-located at each of the spatial cell centers, and defined with f_a and g_a by

$$\rho=\sum\nolimits_a f_a=\sum\nolimits_a f_a^{eq} \tag{14}$$

$$\rho\mathbf{u}=\sum\nolimits_a f_a\mathbf{e}_a=\sum\nolimits_a f_a^{eq}\mathbf{e}_a \tag{15}$$

$$p=\frac{\rho c^2}{3} \tag{16}$$

$$\phi=\sum\nolimits_a g_a=\sum\nolimits_a g_a^{eq} \tag{17}$$

The kinematic viscosity ν and the constant part of the diffusion coefficient Eq. (6), $D_0 = M_{AC}\kappa_\phi$, are defined by the following equations, respectively [8, 9]:

$$\nu=\frac{c^2}{3}\left(\tau_f-\frac{\Delta t}{2}\right) \tag{18}$$

$$D_0=\Gamma c^2\left(\tau_g-\frac{\Delta t}{2}\right) \tag{19}$$

where Γ is the parameter to control the number densities of the moving and rest particles in a stationary equilibrium state of g_a^{eq}.

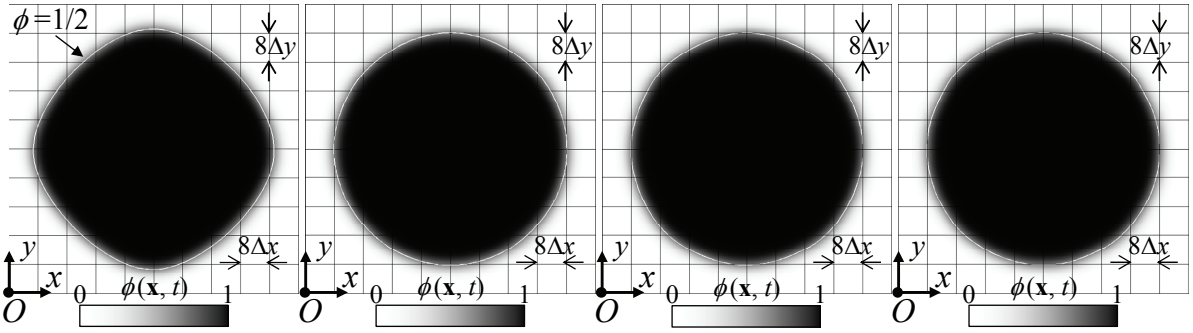
The semi-Lagrangian LBM scheme possesses the advantage over conventional others for directly solving the differential equations, the simple particle-kinematic operation in the discrete conservation form on an isotropic spatial lattice, which is useful for high-performance computational multi-phase fluid dynamics.

4 NUMERICAL RESULTS

4.1 Benchmark test on advection of interface

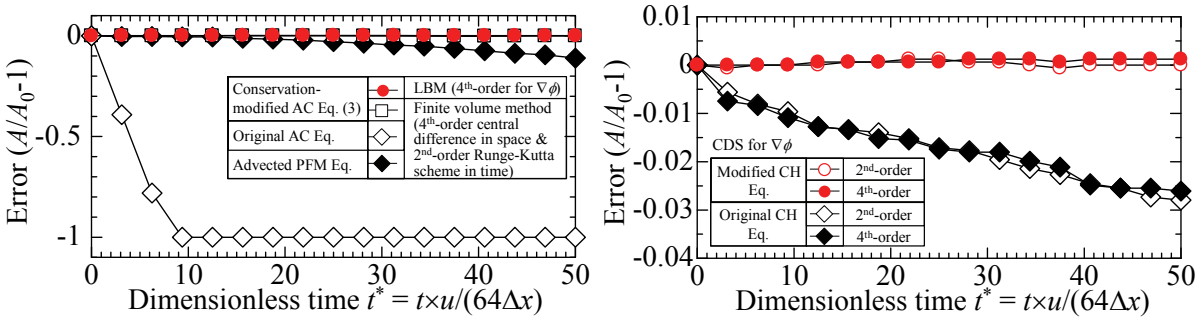
A benchmark test problem of linear translation of a single circular interface in two dimensions (x, y) was solved for evaluating the LBM schemes that we have proposed for the conservation-modified AC and CH equations [8]. The computational domain was uniformly divided into square cells of $200\Delta x \times 200\Delta y$ in a periodic uniform flow with velocity $\mathbf{u} = (u, v)$. The numerical results were obtained under the conditions of $\Delta x = \Delta y = 1$, $\Delta t = 1$, $u = v = 2\times10^{-2}$, and $\kappa_\phi = 1$; this resulted in a Courant number $C = u\Delta t/\Delta x = 2\times10^{-2}$ and theoretical interfacial thickness $4\kappa_\phi^{1/2} = 4$. The value of M_{AC} was selected to be on the same order as that of C for the above Δx, Δt and κ_ϕ, to balance the diffusion with the speed of $M_{AC}\kappa_\phi^{1/2}$ and the advection with $|u|$. To set the initial distribution of $\phi(\mathbf{x},0)$, Equation (3) was iteratively solved under the tentative condition of $\phi = 1$ and 0 inside and outside the circular region with diameters $d = 64$, respectively, to obtain the stationary equilibrium solution. For calculating the interfacial curvature, the gradient of ϕ at each cell center was calculated using a second- or fourth-order central difference scheme (CDS).

The numerical results obtained with the LBM schemes for the modified AC and CH equations are shown in Figs. 1 and 2. In each case of the modified equations, the fluid region advected retains almost its initial shape with the constant interfacial thickness. The initial area of the fluid A_0 has been conserved within 1% error in the modified advection equations better than those in the original equations [7, 8, 14] until dimensionless time $t^* = t\times u/d = 50$. It has been also confirmed that the result obtained with the LBM for the modified AC equation is better than those obtained with finite volume methods adopting second-order central difference schemes in time and second-order Runge-Kutta time-advance scheme [8].



(a) LBM for AC eq. with 2nd-order CDS in grad.ϕ (b) LBM for AC eq. with 4th-order CDS in grad.ϕ (c) LBM for CH eq. with 2nd-order CDS in grad.ϕ (d) LBM for CH eq. with 4th-order CDS in grad.ϕ

Figure 1: Interface-profile solutions of conservation-modified AC and CH equations solved with LBMs after linear translation at dimensionless time $t^* = t\times u/d = 50$ at Courant number $C = u\Delta t/\Delta x = 2\times10^{-2}$ for $d = 64\Delta x$ [8]



(a) Numerical results for conservation-modified AC, original AC and advected PFM equations

(b) Numerical results for modified and original CH equations solved by use of LBM scheme

Figure 2: Area conservation error in linear translation using LBMs for modified and original AC and CH equations at $C = u\Delta t/\Delta x = 2\times10^{-2}$ for $d = 64\Delta x$ [7, 8, 14]

4.2 Two-phase slug flow in rectangular microchannel with T-junction

In advance of two-phase flow simulation, the interfacial tension γ was verified through a preliminary three-dimensional simulation of single droplet neutrally-buoyant in a quiescent continuous liquid phase [9]. In the simulations, the density ρ was initially set at 1.0 uniformly in the whole computational domain, where the continuous and dispersed phases were regarded as the regions with $\phi = 0$ and 1 respectively. Figure 3 shows the difference in pressure Δp between the inside and outside of the suspended spherical droplet with radius R under no gravity. The numerical results agree well with the theoretical predictions by the Laplace's law $\Delta p = 2\gamma/R$ and the definition of γ.

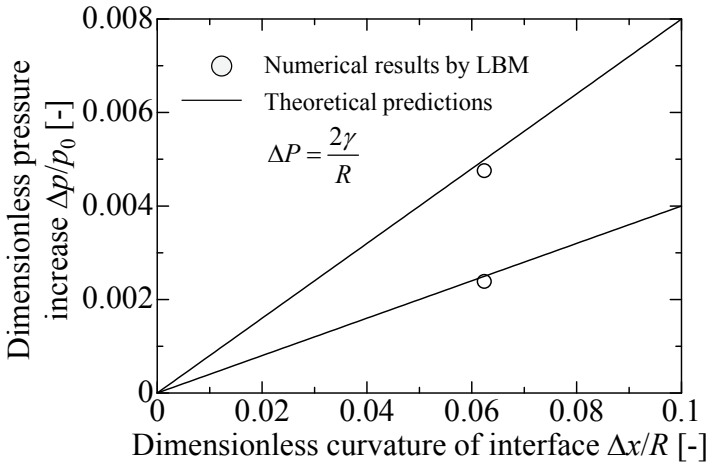


Figure 3: Laplace pressure of spherical droplet with a radius R suspended in quiescent liquid [9]

For developing a novel micro-fabrication process of flexible and large-area sheet display device [1], immiscible liquid-liquid two-phase slug droplets formation in a T-junction microchannel [13] with square cross section and hydrophilic solid walls was investigated through CFD simulation using the PFM and LBM-based method [8, 9]. The continuous and

dispersed phases were assumed as pure water and silicone oil respectively at room temperature, which flow in the channel with square cross section and fully-hydrophilic solid wall surfaces. The volumetric flow rates of the continuous and dispersed phases, Q_W and Q_O, were set in the range of low capillary, Reynolds and Weber numbers respectively, for the two-phase fluid system with hydraulic diameter w of 100 μm, kinematic viscosity ν of 1.0 cSt. and interfacial tension γ of 41.6 mN/m. As shown in Fig. 4, mono-dispersed slug flow pattern is formed in the channel. Figure 5 shows the variation in length and interval of the droplets, L_O and L_W, for the continuous-phase capillary number $Ca_W = \rho\nu(Q_W/w^2)/\gamma$, where $\mu_W = \rho\nu$ is the viscosity. The droplets and their intervals become shorter as both the continuous and dispersed-phase flow rates are increased at a constant ratio of the flow rates $Q_O/Q_W = 1$. It is also confirmed that both the droplet lengths and their intervals in the present simulation agree well with experimental data [9].

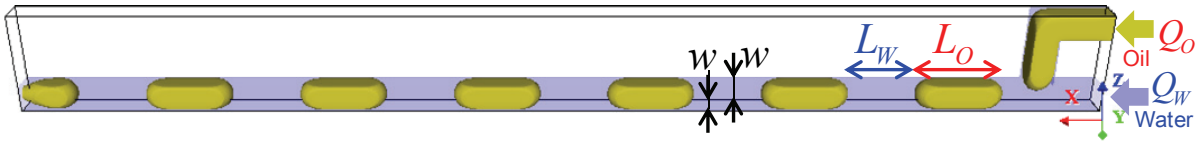


Figure 4: A snapshot of two-phase slug droplets formation in microchannel with T-junction and with square cross-sectional area w^2 at volumetric flow rate ratio $Q_O/Q_W = 1$ for $Ca_W = 2.53\times10^{-4}$ [9].

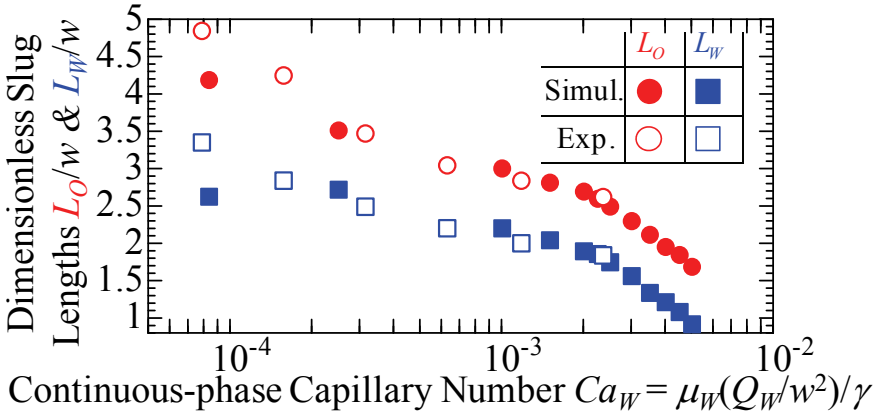


Figure 5: Variations in length of silicone oil L_O and water L_W for capillary number Ca_W at $Q_O/Q_W = 1$ [9].

5 CONCLUSIONS

In this study, Allen-Cahn (AC) and Cahn-Hilliard (CH)-type diffuse-interface advection equations based on a phase-field model (PFM) [3] were evaluated respectively for computational fluid dynamics (CFD) simulations of motion of microscopic two-phase fluid on solid surface. The PFM-CFD method [8, 9] adopting a lattice Boltzmann method (LBM) [10, 11] for solving Navier-Stokes equations with an AC equation [7, 12] was applied to an immiscible liquid-liquid two-phase slug flow problem in a T-junction microchannel [1, 13] with square cross section and hydrophilic solid-wall surfaces.

The following major findings were obtained:

- The use of the LBM schemes allows the initial interfacial shape and volume of a fluid to be adequately retained during translation of the fluid on a spatial structured grid.
- The modified AC and CH advection equations improve the volume-of-fluid conservation much better than the original equations, respectively, by eliminating the interfacial curvature-induced volume flux from the diffusion term which causes the autonomous diffuse-interface formation.
- The PFM-CFD method predicted well the increase in pressure proportional to interfacial curvature inside neutrally-buoyant spherical droplet in agreement with the theoretical prediction according to the Laplace law.
- The method predicted the mono-dispersed slug flow patterns in the channel in good agreement with the experimental data, in terms of decreasing in the length and the interval of the dispersed-phase droplets as increasing both the continuous- and dispersed-phase flow rates at the ratio = 1.

The above-mentioned results prove that the conservation-modified advection equations and the PFM-CFD method [8, 9] will be useful for numerically analyzing the two-phase fluid motions in various micro-fluidic devices and microfabrication processes for MEMS-IC integration [1, 2].

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REFERENCES

[1] Matsumoto, S., Takada, N. and Matsumoto, J. Microfabrication process of cellular structures in hollow fiber-shaped substrates. *Transactions of the Japan Society of Mechanical Engineers Series C*. (2010) **76**: 1911–1913.

[2] Lu, J., Takagi, H., Nakano, T. and Maeda, R. Size-free MEMS-IC high-efficient integration by using carrier wafer with self-assembled monolayer fine pattern. *Proceedings of ECTC2013*. (2013) CFP13ECT-USB: 1508–1513.

[3] Anderson, D. M., McFadden, G. B. and Wheeler, A. A. Diffuse-interface methods in fluid mechanics. *Annu. Rev. Fluid Mech.* (1998) **30**: 139–165.

[4] Takada, N. and Tomiyama, A. A numerical method for two-phase flow based on a phase-field model. *JSME Int. J. Ser. B – Fluids Therm. Eng.* (2006) **49**: 636–644.

[5] Matsumoto, J. and Takada, N. Two-phase flow analysis based on a phase-field model using orthogonal basis bubble function finite element method. *Int. J. Comput. Fluid Dyn.* (2008) **22**: 555–568.

[6] Takada, N., Matsumoto, J., Matsumoto, S. and Ichikawa, N. Application of a phase-field method to the numerical analysis of motions of a two-phase fluid with high density ratio on a solid surface. *Journal of Computational Science and Technology*. (2008) **2**: 318–329.

[7] Chiu, P.-H. and Lin, Y.-T. A conservative phase field method for solving incompressible

two-phase flows. *J. Comput. Phys.* (2011) **230**: 185–204.

[8] Takada, N., Matsumoto, J. and Matsumoto, S. Phase-field model-based simulation of motions of a two-phase fluid on solid surface. *Journal of Computational Science and Technology*. (2013) **7**: 322–337.

[9] Takada, N., Matsumoto, J. and Matsumoto, S. A diffuse-interface tracking method for the numerical simulation of motions of a two-phase fluid on a solid surface. *Proceedings of the 8th International Conference on Multiphase Flow*. (2013) Paper ID: **ICMF2013-599**.

[10] Chen, S. and Doolen, G. D. Lattice Boltzmann method for fluid flows. *Annu. Rev. Fluid Mech.* (1998) **30**: 329–364.

[11] Inamuro, T., Ogata, T., Tajima, S. and Konishi, N. A lattice Boltzmann method for incompressible two-phase flows with large density differences. *J. Comput. Phys.* (2004) **198**: 628–644.

[12] Olsson, E. and Kreiss, G. A conservative level set method for two phase flow. *J. Comput. Phys.* (2005) **210**: 225–246.

[13] Garstecki, P., Fuerstman, M., Stone, H. and Whitesides, M. Formation of droplets and bubbles in a microfluidic T-junction – scaling and mechanism of break-up. *Lab Chip* (2006) **6**: 437–446.

[14] Beaucourt, J., Biben, T., Leyat, A. and Verdier, C. Modeling breakup and relaxation of Newtonian droplets using the advected phase-field approach. *Phys. Rev. E.* (2007) **75**: 021405.