CFD SIMULATION OF TWO-PHASE FLUID FLOWS
USING A PHASE-FIELD MODEL

Naoki Takada, Junichi Matsumoto and Sohei Matsumoto
National Institute of Advanced Industrial Science and Technology (AIST)
1-2-1 Namiki, Tsukuba-shi, Ibaraki 305-8564, JAPAN

1. Introduction
Gas-liquid and liquid-liquid flows with a fluid-fluid interface are widely encountered in various fields of science and engineering. In the flows, bubbles and droplets are advected, deformed, break up into smaller ones and coalesce with each other. Computational fluid dynamics (CFD) simulations facilitate the understanding and prediction of such two-phase flow phenomena; as its result, fluidic devices and machineries, manufacturing processes and power plants can be optimized for flexible and accurate flow control. It is often difficult to experimentally observe such flows and measure the scalar and vector variables simultaneously in three dimensions or to analyze theoretically them by the classical continuum-dynamics approach using a sharp-interface model. Therefore, it is important to develop CFD methods for analyzing the flow phenomena.

In recent years, phase-field model (PFM) has grown popular as one of useful tools for the understanding and prediction of complex phenomena involving self organization of mesoscopic structures in multi-component systems, such as two-phase flows, solidification of binary alloys and formation of polymer membranes. Based on the van-der-Waals, Cahn-Hilliard free-energy theory, PFM describes an interface as a volumetric transition zone with a finite width between pure components (phases), across which physical properties vary steeply but continuously. The coexistence of two phases with the diffusive interface is allowed by a free-energy functional which has a double-well potential of an order parameter (mass density or molar concentration) and depends on square of its local gradient, without imposing topological constraints on interface as phase boundary. In the theory, surface tension is defined as an excessive free energy per unit area caused by local gradient of the order parameter inside the interface zone, enabling calculation of the continuous body force without using interfacial curvature and normal vector. As a result, the PFM-based CFD method for two-phase flows does not necessarily require conventional elaborating algorithms for advection and reconstruction of interface and continuum surface force modeling in front-tracking, level-set and volume-of-fluid (VOF) methods. This feature simplifies interface-tracking calculation on a fixed spatial grid. The PFM method therefore has attractive advantages over the other methods, easy implementations of multi-dimensional advection of interface and associated heat and mass transfer across the interface.

The PFM methods are categorized into two types; a direct numerical method using Navier-Stokes (NS) equations (NS-PFM), and a lattice Boltzmann method (LBM) using mesoscopic kinetic equations for the velocity distribution of a number density of fictitious fluid particles. Both types had been applied only to two-phase flows with a small density difference because of numerical instability. To overcome the difficulty, two kinds of two-phase LBM proposed by Chen et al. and Inamuro et al. adopted conventional finite difference scheme for problems with contact discontinuity and solution algorithm for Poisson equation of pressure, respectively. Based on the latter LBM, we have recently proposed a NS-PFM applicable to two-phase flow problems at a high density ratio. One of advantages of NS-PFM over two-phase LBM is to save computational memory, because the number of macroscopic variables in NS equations is generally less than that of mesoscopic variables (particle-velocity distribution functions) in the LBM kinetic equations. On the other hand, LBM has the advantage of simple algorithm of motions of the particles, their linear translations with constant velocities and local mass- and momentum-conserving collisions with each other.

In the presentation, CFD simulation results of isothermal and thermal two-phase fluid flows by the PFM-based methods will be shown for discussion of the applicability to the flow problems.
2. CFD simulation of two-phase flow by using phase-field model

Two kinds of isothermal two-phase flow simulations using PFM are briefly described hereafter. For examining the applicability of the NS-PFM to motions of two-phase fluid with high density ratio, we first applied it to the collapse of a two-dimensional liquid column in a gas under gravity \( g \) in a rectangular domain surrounded with neutrally wettable solid walls (contact angle \( \theta_W = 90^\circ \)). The contact angle, depending on the free-energy balance among three types of 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. The initial column width \( a = 40 \) spatial square cells was assumed to be equivalent to 2.25 inches in the air-water system. The effect of \( g \) on the fluid was taken into account only in the gas-phase regions. As shown in Fig. 1 at dimensionless time \( t_1^* = t(2|g/a|^{0.5}) \) for aspect ratio of the column \( H/a = 2 \), the liquid column collapses and the interface slides on the bottom solid wall to the right side wall. We have confirmed that time histories of the leading-edge position and the height of the column agree with available data.

One of the applications to capillary-force flow problem is to three-dimensional displacement and breakup motions of a single droplet on a flat solid surface in a stagnant gas under no gravity. This simulation was conducted for preliminarily examining the fundamental capability of the NS-PFM to predict the motions of bubbles or droplets in micro-fluidic devices that control them at high frequency by using electro-wetting-on-dielectrode (EWOD) technology. On the bottom solid wall, a droplet of mass density \( \rho_L \) and surface tension \( \sigma \) was initially formed with a hemispherical shape with radius \( R = 16 \) spatial cells in the stagnant gas. It was assumed that the fluids were air and water and \( R = 8 \) mm. Hydrophilic surface regions were located on both sides of hydrophobic region with width \( a = R \) on the central part of the bottom wall surface.

**Figure 2** shows the shape of the droplet at each dimensionless time \( \tilde{t} \) for difference between static contact angles on the solid surface, \( \Delta \theta_W = 86^\circ \). The droplet breaks up into a pair of twin droplets, and a tiny satellite droplet is also generated between them from a throat part of the parent droplet that is deformed to have a dumbbell-like shape. The results of the droplet motions driven by the difference in capillary force are well predicted qualitatively in comparison with the experimental observation of a water droplet in a micro channel and other numerical results.

**Publication**