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Numerical simulations of spontaneous capillary rises with very low capillary numbers using a front-tracking method combined with generalized Navier boundary condition

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ABSTRACT

We propose a front-tracking method that considers a moving contact line with a generalized Navier boundary condition (GNBC) and with a delta function distribution approximated on the grid scale. A method of evaluating the interfacial balance at the contact line in the form of a body force, which is straightforward with the front-tracking method, cannot give a natural flow field. In contrast, the proposed method using the GNBC, which includes the unbalanced Young's force as stress on the wall, can give a very stable and reasonable flow field. The proposed front-tracking method was applied for the capillary rise of a liquid in a tube, in which the velocity-dependent contact angle dominates the dynamic characteristics. The validity of the proposed method was confirmed by comparing simulation results with experimental measurements and simple theoretical models. The results of the present simulations with adjusted non-dimensional slip parameters agreed very well with experimental measurements. Under the present simulation conditions, the linearity of the GNBC allows the correlation between the dynamic contact angle and the contact line's velocity to follow a simple linear expression that involves the difference of the cosine with the capillary number. The non-dimensional slip parameter, which represents the dynamic nature of the moving contact line, can therefore be easily adjusted to reproduce experimental observations under small-capillary-number conditions.

1. Introduction

1.1. Moving contact line

The wetting of a solid surface by a liquid is not only a physically interesting phenomenon but also a very important issue in many industrial processes. When a liquid–gas interface touches a solid surface, a three-phase contact line forms; the static contact angle (i.e., the equilibrium angle between the solid–liquid and liquid–gas interfaces at the contact line) is often used to describe the wettability of the solid surface. When wetting or dewetting occurs, the contact line moves and the contact angle changes dynamically. The dynamics of the moving contact line is related to the dynamic contact angle, which has been studied by various researchers (Dussan, 1979; Adamson, 1990; Brochard-Wyart and de Gennes, 1992; Blake, 1993; Kistler, 1993; Shikhmurzaev, 2007).

In fluid dynamics, a solid surface is generally represented by a no-slip boundary at which the fluid velocity is zero relative to the solid. However, the no-slip boundary condition fails at the contact line because of a non-integrable singularity in the viscous stress, as found in the analytical solution by Huh and Scriven (1971). To describe the moving contact line theoretically, two approaches have been used: first that uses hydrodynamics and second that uses molecular kinetics. Using the first approach, Voinov (1976) divided the flow field into microscopic and macroscopic scales, following which Cox (1986) introduced an intermediate scale between these two scales. Both Voinov and Cox permit liquid slip on the solid surface in the microscopic region very close to the contact line. The relations between the dynamic contact angle and the slip velocity are then derived by matching asymptotic expansions. De Gennes (1986) derived similar velocity–angle correlations by considering the viscous dissipation in the contact-line region. With the second approach, Blake and Haynes (1969), Hoffman (1983), and Blake (2006) derived the correlation between the dynamic contact angle and the contact-line velocity from molecular theories by considering the adsorption–desorption process very near to the contact line. Both the hydrodynamics and molecular kinetics approaches can be made to fit a number of experimental results (e.g. Hoffman, 1975; Tanner,

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1979), which means that the essential mechanism of the moving contact line is not fully understood.

1.2. Numerical simulations

Numerical simulation is a powerful tool for analyzing multiphase systems and has been applied to various systems. Renardy et al. (2001) treated the moving-contact-line problems with the volume-of-fluid (VOF) method. However, their model of the moving contact line is not based on physical concepts but rather on the strategy of implementing VOF method with fixed static contact angles. In a general staggered grid system and for finite-difference calculations, the velocity tangential to the wall and the volume fraction are not placed on the solid surface; thus, despite the no-slip boundary condition, the contact line moves at the velocity of the liquid at a half-grid apart from the wall. Šikalo et al. (2005), Fang et al. (2008), Afkhami et al. (2009), Schönfeld and Hardt (2009), and Dupont and Legendre (2010) also simulated the moving-contact-line problems with the VOF method. All of their simulations used empirical relations between the dynamic contact angle and the moving-contact-line velocity, to predetermine the contact angle via the moving velocity or vice versa.

Spelt (2005), Mukherjee and Knadlikar (2007), and Yokoi et al. (2009) approached the problem with the level-set method. For moving contact lines, they used a classical Navier boundary condition (NBC) (Huh and Mason, 1977; Qian et al., 2006), which assumes that the slip velocity is proportional to the velocity gradient near the wall. In these simulations, the contact angles or the contact-line velocities are still prescribed by the empirical relations.

In another approach, Zahedi et al. (2009) represented the moving contact line by artificial diffusion in the re-initialization process of the level-set method. Yet other researchers used the Cahn–Hilliard theory to describe the moving contact line by the diffused interface (Seppecher, 1996; Jacqmin, 2000; Takada et al., 2008) or the lattice Boltzmann method (Briant et al., 2004; Yan and Zu, 2007). These methods (Seppecher, 1996; Jacqmin, 2000; Takada et al., 2008; Briant et al., 2004; Yan and Zu, 2007) also represent the moving contact line by interface diffusion.

Besides the finite-element method (Baer et al., 2000), other methods used to represent the moving contact line are the hybrid method that combines molecular dynamics simulation and finite elements (Hadjiconstantinou, 1999a,b), the sharp interface method (Liu et al., 2005), and the front-tracking method (Huang et al., 2004).

1.3. Slip evidence by molecular dynamics simulations

For single-phase systems, Thompson and Troian (1997) conducted a molecular dynamics (MD) simulation and confirmed the validity of the NBC, which assumes that the drag force due to slip is proportional to the viscous stress on the wall [Eq. (14)]. In general, the constant slip coefficient is a good approximation. Before the work by Thompson and Troian, slip at the solid surface for two-phase systems was studied by Koplik et al. (1988, 1989), Thompson and Robbins (1989), and Thompson et al. (1993). Their MD studies provided clear evidence that the no-slip boundary condition breaks down in a region near the contact line. Through careful MD studies, Qian et al. (2003) provided convincing evidence that the interfacial Young's stress dominates in the contact-line region. Based on a force-balance argument, Qian et al. proposed the generalized Navier boundary condition (GNBC), which accounts for the uncompensated (or unbalanced) Young's stress in the contact line region (described in Section 2.2.1). In addition, they originally proposed the GNBC for the diffused interface method and confirmed its validity. Ren and Weinan (2007) applied a model analogous to the GNBC for an immersed-boundary-type simulation. Gerbeau and Lelièvre (2009) incorporated the GNBC in an arbitrary Lagrangian–Eulerian (ALE) framework. Ito et al. (2008) combined the GNBC into the theoretical approach by Huh and Scriven (1971) and by comparing with their own MD results, confirmed that its results are very reasonable.

1.4. Objectives

The front-tracking approach of Huang et al. (2004) represented the interface by connected marker points. They used this approach to evaluate the interface curvature for interfacial tension forces by differentiating the approximated curve. The original front-tracking method by Tryggvason's group (Tryggvason et al., 2001), however, evaluated the tangential pulling forces of each element. This latter approach offered a great advantage when the interface of the two fluids connects with another fluid (or solid) surface. For the VOF, level-set, diffused interface, or similar implicit-interface methods, continuum surface force (CSF)-type models (Brackbill et al., 1992) are often used to evaluate the surface tension force from the curvature of the indicator function. However, at least one phase surface (e.g., the liquid surface in Fig. 1) forms a cusp at the triple junction, in which case the curvature approach cannot represent the correct shape and results in an unstable flow field, as shown in Renardy et al. (2001). Thus, for stable calculations in methods that involve curvature and for the wetting of a solid surface, the surface shape that corresponds to the contact angle must be predetermined. However, the front-tracking approach, which evaluated the tangential pulling force at both element ends (as described in Section 2.2 and Fig. 1), correctly represented the force balance even at the triple junction between three fluids, as confirmed in Yamamoto and Uemura (2008). The front-tracking method without curvature evaluation does not need to predetermine the contact angle; the complete interface shape can be calculated explicitly by the velocity field of the fluid.

Herein, we propose a simulation method to represent the wetting of solid surface based on the front-tracking method. In the front-tracking method, interface markers accurately represent interfacial tensions even at the contact line, so the contact angle need not be predetermined. For a moving contact line, the GNBC proposed by Qian et al. is combined in a form suitable for the front-tracking method. In this form, the delta-function-type

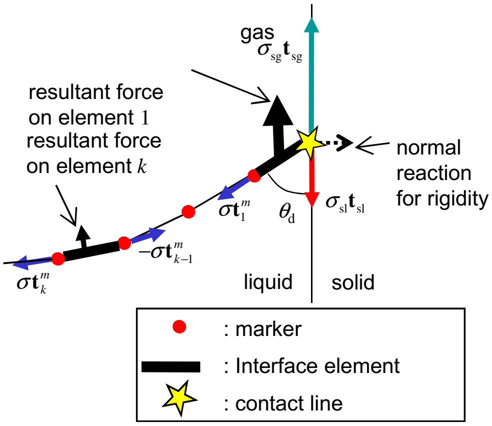

Fig. 1. Interfacial tension effect represented by the marker-connected element for gas–liquid interface and for interface that contains contact line (for a straightforward representation in three-phase front-tracking). σ, σ_{sl} and σ_{sg} are the interfacial tensions between gas–liquid, solid–liquid, and solid–gas, respectively. $\boldsymbol{t}_k^m$ is the unit tangent at the kth marker point, and $\boldsymbol{t}_{sl}$ and $\boldsymbol{t}_{sg}$ are the unit tangents of the solid–liquid and solid–gas interfaces at the contact line.