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Modeling of the dynamic wetting behavior in a capillary tube considering the macroscopic–microscopic contact angle relation and generalized Navier boundary condition

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ABSTRACT

In this study, dynamic wetting phenomena in a capillary tube were studied by using numerical simulations based on the front-tracking method employing the generalized Navier boundary condition (GNBC) and by experimental measurements. For the GNBC, based on molecular dynamics simulations, the microscopic dynamic contact angle is estimated from the grid-scale contact angle using Cox's macroscopic–microscopic relation. The experimentally measured correlation between the apparent dynamic contact angle and the moving velocity of the contact line is well reproduced by the present simulation technique considering Cox's macroscopic–microscopic relation. Thus, we found that the dynamics of wetting are well described by combining molecular-scale behavior and macroscopic–microscopic relations.

1. Introduction

The wetting of a solid surface by a liquid is not only a physically interesting phenomenon but also critical in many industrial processes. 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 (e.g., see reviews by de Gennes, 1985; Bonn et al., 2009). In general, in continuum fluid dynamics, a solid surface is treated as a no-slip boundary. However, the contact line never moves (wetting or dewetting never occurs) and viscous stress diverges under the no-slip boundary condition. To reasonably represent the moving contact line, we have developed a new method on the basis of the generalized Navier boundary condition (GNBC) proposed by Qian et al. (2003) and combined it with the front-tracking method (Yamamoto et al., 2013). By using the grid-scale slip, the divergence of the viscous stress is avoided, and the experimentally observed dynamic properties can be well reproduced for very low capillary number conditions.

Yamamoto et al. (2013) considered the conditions for contact angles near 90° and small capillary numbers $O(10^{-3})$. In this paper, the conditions for very small contact angles and rather large capillary numbers are considered, and a dynamic wetting model is proposed and evaluated.

The GNBC model (Qian et al., 2003) is constructed on the basis of molecular dynamics (MD) simulation results. Based on a force-balance argument through careful MD studies, Qian et al. provided convincing evidence that the interfacial Young's stress still dominates the dynamic force balance in the region molecularly vicinity of the contact line. Therefore, the dynamic contact angle used in the GNBC is a microscopically (nm order) observed angle. However, we can obtain the grid-scale (μm∼mm order) macroscopic contact angle in the front-tracking simulation with practical resolution. In some conditions (e.g., very low capillary number) reported by Yamamoto et al. (2013), the microscopic and macroscopic contact angles do not differ much; however, in general, they differ according to the analysis by Cox (1986). Thus, we introduce a new method that combines Cox's macroscopic–microscopic angle relation and the GNBC. In this method, the microscopic dynamic contact angle is estimated from Cox's relation and used in the GNBC for computing the moving contact line. To date, similar modeling efforts have been proposed for representing

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the unresolved microscopic behavior. For example, Afkhami et al. (2009) used an approximation of Cox's relation, Dupont and Legendre (2010) used a similar relation by Ngan and Dussan (1989), Sui and Spelt (2013) used Cox's relation with higher order. However, all of them consider a fixed static contact angle as a microscopic contact angle. Sui and Spelt (2013) compared their simulations with experimental data and showed that considering the microscopic contact angle as static leads to unrealistic microscopic length scales. In the proposed method, the unresolved microscopic behavior is treated in macroscopic scale simulations using Cox's relation. However, we considered a dynamic microscopic angle and applied the GNBC model to a microscopic dynamic contact angle and slip velocity relation. Unlike the hybrid method that combines molecular dynamics simulation and finite elements by (Hadjiconstantinou, 1999a,b), we use the GNBC just as a slip boundary condition. In addition, we compared the simulation results with experimental data and discuss the model parameters.

2. Numerical method

2.1. Front-tracking method

In the front-tracking method (Unverdi and Tryggvason, 1992), the gas–liquid interface is tracked by marker points and the interface information is calculated by elements connecting markers. Using this information, the single-fluid equations are solved by using the finite-difference method. In this study, the calculation was performed on the staggered grid system and axisymmetric cylindrical coordinate system, where x is the radial (horizontal) and y is the axial (vertical) direction. The velocity components are represented by u and v in the x- and y-direction, respectively.

2.2. Generalized Navier boundary condition (GNBC)

The GNBC was proposed by Qian et al. (2003) on the basis of MD simulations. One piece of evidence is that the tangential interaction force between the fluid molecules in a very thin layer adjacent to a wall and the wall molecules is proportional to the slip velocity. Another piece of evidence is that the interaction force acting on the very thin layer adjacent to the wall can be represented by the viscous shear stress on the wall $\tau_{\rm wall}^{\rm visc}$ and unbalanced Young's stress $\widetilde{\tau}^{\rm Young}$. The GNBC can then be represented as

$$\beta v_{\rm slip} = \tau_{\rm wall}^{\rm visc} + \widetilde{\tau}^{\rm Young}, \tag{1}$$

where $v_{\rm slip}$ is the slip velocity on the wall and β is the slip coefficient. Unbalanced Young's stress is given by the integral,

$$\int_{\rm int} \widetilde{\tau}^{\rm Young}\, dy = \sigma(\cos\theta_{\rm s} - \cos\theta_{\rm d}), \tag{2}$$

where $\theta_{\rm s}$ and $\theta_{\rm d}$ are the static and dynamic contact angle, respectively, σ is the surface tension of the liquid, and the integration is applied across the diffused interface along the direction parallel to the wall. Yamamoto et al. (2013) proposed a numerical implementation of the stress by an approximation of the delta function used in the front-tracking method,

$$\widetilde{\tau}^{\rm Young}(y_j) = \sigma(\cos\theta_{\rm s} - \cos\theta_{\rm d})d(y_j - y_{\rm cl}), \tag{3}$$

where y_j and $y_{\rm cl}$ are the positions of the jth grid point and the contact line, respectively. The approximated delta function d proposed by Peskin (2002) is given by,

$$d(r) = \begin{cases} \dfrac{1}{4\Delta}\left(1+\cos\dfrac{\pi r}{2\Delta}\right), & |r| \leqslant 2\Delta, \\ 0, & |r| > 2\Delta, \end{cases} \tag{4}$$

where Δ is the grid spacing. $\theta_{\rm d}$ is calculated by the three-marker-point Lagrangean approximation. Then, $v_{\rm slip}$ is obtained from Eq. (1) with Eqs. (3) and (4), and used as the boundary conditions on the wall.

2.3. Simplification of GNBC

Using the GNBC, the divergence of the viscous stress is avoided because the large slip velocity occurs at the contact line. Moreover, owing to the decrease in the viscous stress, the first term of the right-hand side of Eq. (1) is negligible compared with the second term. Thus, only the slip velocity due to unbalanced Young's stress near the contact line is accounted in Eq. (1). In the region far from the contact line, the no-slip condition is applied. We refer to this boundary condition as the simplified GNBC (SGNBC). In the conditions considered in this study, there is no significant difference between the SGNBC and GNBC in the simulations. The same type of slip models was also considered by Ren and E (2007).

By using the SGNBC, the nondimensional contact line velocity (i.e., capillary number $Ca \equiv \mu v_{\rm cl}/\sigma$, where μ is the viscosity of the liquid phase and $v_{\rm cl}$ is the contact line velocity corresponding to $v_{\rm slip}(y_{\rm cl})$) is derived by Eqs. (1), (3), and (4) with $y = y_{\rm cl}$ and neglecting $\tau_{\rm wall}^{\rm visc}$,

$$Ca = \chi(\cos\theta_{\rm s} - \cos\theta_{\rm d}), \tag{5}$$

where $\chi(=\bar{\mu}/(\beta\Delta))$ is the nondimensional slip parameter that represents the dynamic property of wetting. $\bar{\mu}$ is the arithmetic average viscosity, and this treatment is discussed in the electronic Annex 1 in the online version of the Yamamoto et al. (2013) study. Because we use resolution-dependent distributions of the interfacial information in the front-tracking procedure, Eq. (3) also depends on the grid resolution Δ. Thus, slip coefficient β is no longer a physical parameter, and parameter χ should be treated as the nondimensional slip parameter as confirmed by Yamamoto et al. (2013). It is found from Fig. 9(a) and (b) in Yamamoto et al. (2013) that Young's stress is much larger (100 times or more) than viscous stress at the contact line with any resolution. And it is found from Fig. 13 in Yamamoto et al. (2013) that the capillary number is perfectly proportional to cosine of the dynamic contact angle in the same manner as Eq. (5). So we consider that the viscous term in the GNBC can be neglected.

Eq. (5) represents the slip related to the deviation of the instantaneous contact angle from the static contact angle, and the contact line moves making the contact angle to approach the static contact angle. The parameter χ characterizes the response time of the contact line movement. A large χ results in large Ca and then the contact angle rapidly approaches the static angle. Then, the wall slip velocity is given in the form using Ca from Eqs. (1), (3), (5) and delta function distribution $2\Delta d$ as

$$v_{\rm slip}(y_j) = Ca\frac{\sigma}{\mu}2\Delta d(y_j - y_{\rm cl}). \tag{6}$$

2.4. Estimation of the microscopic contact angle using Cox's relationc

Because the GNBC is constructed on the basis of MD simulations, the dynamic contact angle in Eq. (5) should be microscopically measured as

$$Ca = \chi(\cos\theta_{\rm s} - \cos\theta_{\rm d}^{\rm micro}). \tag{7}$$

However, in the front-tracking method, the obtained contact angles are macroscopically measured in the grid scale (marker intervals are between 0.6Δ and 0.8Δ). Therefore, we used the relation between the macroscopic contact angle $\theta_{\rm d}^{\rm macro}$ and the microscopic angle $\theta_{\rm d}^{\rm micro}$ derived by Cox using the matched asymptotic expansion (Cox, 1986)

$$G(\theta_{\rm d}^{\rm macro}) = G(\theta_{\rm d}^{\rm micro}) + Ca\ln\left(\frac{l^{\rm macro}}{l^{\rm micro}}\right) + O(Ca), \tag{8}$$