

Simulation of moving contact lines in two-phase polymeric fluids



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ABSTRACT

We numerically study the influence of polymer additives on contact line dynamics using a sharp interface model. An additional term, which accounts for the polymer stress, is added to the two-phase Navier–Stokes equation. The polymer stress is modeled by the FENE-P model. The coupled dynamic equations are solved using the finite difference method. The interface is tracked using marker particles, and the interface conditions are imposed using the immersed boundary method. Simulations in a Couette geometry are carried out to study the effect of the polymer stress on the moving contact line. It is found that the large velocity gradient near the moving contact line results in large polymer stress, which retards the contact line motion. The polymer stress increases with the polymer viscosity but is insensitive to the change of the Weissenberg number. The strength of the polymer stress is also found to increase with the capillary number, especially when the capillary number is large. We also study the relation between the apparent contact angle and the capillary number. For Newtonian fluids, the relation fits well with Cox's analytic result; however deviation occurs for polymeric fluids. The critical capillary number at which the transition to an unsteady state happens decreases as the polymer viscosity increases.

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1. Introduction

A moving contact line is formed when one fluid displaces another fluid on a solid surface (see Fig. 1). Understanding the contact line dynamics is important to many industrial applications such as coating, contact dispensing, inkjet printing, spray cooling, and the application of agrochemicals [1–4]. While the contact line dynamics in Newtonian fluids has been extensively studied [5–11], the influence of additives such as nanoparticles, surfactants and polymers on contact line dynamics is less understood [4,12,13]. These additives can influence the contact line dynamics via a variety of mechanisms, e.g. pinning of the contact line, changing the surface tensions of the fluid/fluid or fluid/solid interfaces, or the viscosity of the fluids, etc. In this work, we focus on the influence of the polymer stress on the moving contact line.

It is well known that when the moving contact line is modeled using the classical hydrodynamics with the no-slip boundary condition, the stress has a non-physical singularity at the contact line with infinite rate of energy dissipation [14,15]. To overcome this difficulty, a number of regularized models have been proposed. These include the slip models [16–21], phase-field models [22–24], and others [7,25]. In this work, we use the slip model derived by Ren et al. [20,26]. The boundary con-

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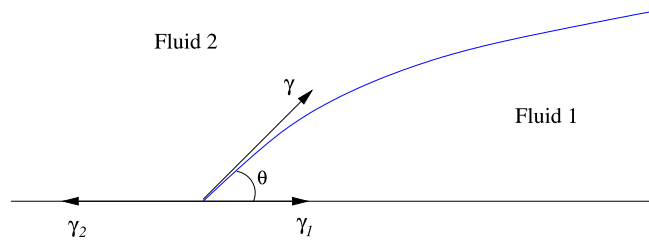


Fig. 1. Two immiscible fluids in contact with a solid substrate. γ , γ_1 and γ_2 are the surface tension coefficients of the three interfaces; θ is the contact angle of the fluid interface with the solid surface.

ditions in this model were derived based on thermodynamics principles and molecular dynamics simulations. In this work, we incorporate a polymer stress into the model and study the influence of polymer additives on the contact line dynamics.

In polymeric fluids, the flow is coupled with polymer dynamics: the flow field deforms the polymer chains from their equilibrium configuration; the deformation of the polymer chains in turn results in a force acting on the flow. The effect of this interaction on the contact line dynamics has been examined in a number of experiments. For example, Min et al. [27] studied the relation between the apparent contact angle and the contact line speed in the wetting dynamics of a polymer fluid. Ramé et al. [28] carried out a series of experiments for the spreading of a polydimethylsiloxane liquid, and found that the length scale and the microscopic contact angle that characterize the physics near the contact line have a detectable dependence on the spreading velocity. They attributed these phenomena to the additional time scale caused by the elasticity of the polymers near the moving contact line. In the study of the wedge flow of non-Newtonian fluids near the contact line, Wei et al. [29] found shear thinning has a strong effect on the wetting dynamics; in contrast, the dynamics is insensitive to the elasticity of the fluid. In addition to dynamic wetting, there were also some experiments studying the influences of polymer additives on the dynamics of a drop impacting a solid surface. Bergeron et al. [4] observed slow retraction during drop impact and attributed it to the additional energy dissipation caused by the stretching of polymers near the contact line. Smith et al. [30] observed the deposition of polymers on the solid surface during the retraction of a drop of dilute polymer solution. This suggests that polymer additives may affect the contact line dynamics by interacting with the substrate.

A number of numerical methods have been proposed to study the contact line dynamics in Newtonian fluids. These include the level-set method [31–34], the volume-of-fluid method [35–37], the front tracking method [38,39], the phase-field method [40,41], and the immersed boundary method [42]. For viscoelastic fluids, much less numerical study has been done. Yue et al. [43,44] developed a finite element method for a phase-field model. They observed that the polymer stress enhances the bending of the fluid interface if polymers are added to the advancing fluid, and reduces the bending of the interface if polymers are added to the receding fluid.

This paper is devoted to a numerical study of the contact line dynamics in two-phase FENE-P fluids using a sharp interface model. We begin in Section 2 with the mathematical model for the contact line problem in viscoelastic fluids. The sharp interface model is coupled with the FENE-P model for the polymer stress tensor. In Section 3, we develop a finite difference method to solve the coupled equations. In Section 4, we present numerical results. Concluding remarks are made in Section 5.

2. Contact line model for viscoelastic fluids

We assume the fluids are incompressible, so the flow is modeled by the conservation laws for mass and momentum:

$$\rho_i(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{T}, \tag{1a}$$

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

in the bulk Ω_i for $i = 1, 2$. In the above equations, ρ_i ($i = 1, 2$) is the fluid density, T is the stress tensor

$$\mathbf{T} = \mathbf{T}_s + \mathbf{T}_p, \tag{2}$$

where T_s and T_p are the viscous stress of the solvent and the polymer stress, respectively. The viscous stress is modeled using the linear constitutive relation

$$\mathbf{T}_s = \eta_i \mathbf{D} = \eta_i (\nabla \mathbf{u} + (\nabla \mathbf{u})^T), \tag{3}$$

where η_i is the viscosity of the solvent. Different models with various complexity exist for the polymer stress; in this work we use the FENE-P (Finitely Extensible Nonlinear Elastic) dumbbell model [45,46]:

$$\mathbf{T}_p = \frac{\eta_p}{\tau} \left(\frac{1}{1 - \text{tr} \mathbf{A} / E_d} \mathbf{A} - \frac{1}{1 - 3/E_d} \mathbf{I} \right), \tag{4}$$

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