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Energy dissipation due to viscosity during deformation of a capillary surface subject to contact angle hysteresis

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ABSTRACT

A capillary surface is the boundary between two immiscible fluids. When the two fluids are in contact with a solid surface, there is a contact line. The physical phenomena that cause dissipation of energy during a motion of the contact line are hysteresis in the contact angle dynamics, and viscosity of the fluids involved.

In this paper, we consider a simplified problem where a liquid and a gas are bounded between two parallel plane surfaces with a capillary surface between the liquid–gas interface. The liquid–plane interface is considered to be non-ideal, which implies that the contact angle of the capillary surface at the interface is set-valued, and change in the contact angle exhibits hysteresis. We analyze a two-point boundary value problem for the fluid flow described by the Navier–Stokes and continuity equations, wherein a capillary surface with one contact angle is deformed to another with a different contact angle. The main contribution of this paper is that we show the existence of non-unique classical solutions to this problem, and numerically compute the dissipation.

1. Introduction

A capillary surface is the boundary between two immiscible fluids. When the two fluids are in contact with a solid surface, there is a contact line. The physical phenomena that cause dissipation of energy during a motion of the contact line are hysteresis in the contact angle dynamics, and viscosity of the fluids involved. For a specific combination of fluids, these two phenomena might have widely differing contribution to the total energy loss. In this paper, we start our investigation of contact line motion by studying the the dissipation of energy due to viscosity when a capillary surface is deformed from one shape to another due to the motion of the boundary.

1.1. Contact angle hysteresis

Consider a liquid droplet on a solid surface with a contact angle of θ. Experiments show that if the liquid is carefully added to the droplet, the volume and contact angle of the droplet will increase without changing the diameter d of the contact disk until the contact angle reaches a critical value θ_a - called the advancing angle [1]. Similarly, if the liquid is removed from a droplet, volume and contact angle of the droplet decrease, but the contact diameter remains the same until a critical angle called the receding angle θ_r is reached.

Consider a liquid drop, which has a spherical cap shape, on a solid surface. Let V, R, and d be the volume of the drop, the radius of the sphere, and the diameter of the disc which forms the contact region, respectively. Let θ be the contact angle, and δp be the difference in pressure between the inside and outside of the drop. We assume that the drop is small enough that the pressure inside the drop is uniform (that is, the effect of gravity is negligible). Then, we have the equations:

$$\sin(\theta) = \frac{d}{2R}, \quad \delta p = \frac{2\gamma}{R}, \quad V = \frac{2\pi R^3}{3}(1-\cos^3(\theta)),$$

where γ is the surface tension of the liquid. Fig. 1 shows the variation of the contact angle θ with the diameter d, while Fig. 2 shows the variation of (δp) with the volume V is.

The integral $\int \delta p \, dV$ computed on any path in Fig. 2 represents the work that is done either by or on the droplet. Thus, if the droplet begins with a certain contact diameter and contact angle at point A, and the volume is increased until point B is reached, followed by a decrease in volume to points C and D, and then an increase in volume back to point A, then the area of the hysteresis loop ABCDA is the net work that must be done by the droplet (or the external agent) against the surrounding to overcome contact angle hysteresis.

The important point to note is that if the contact line does not move then there is no loss due to contact angle hysteresis. However, there might be losses due to viscous dissipation.

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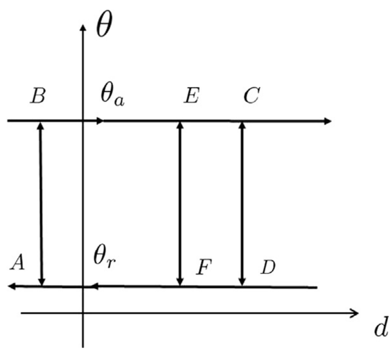

Fig. 1. Plot of the contact angle θ versus contact diameter d for a drop on a solid surface. The advancing angle is θ_a, and the receding angle is θ_r.

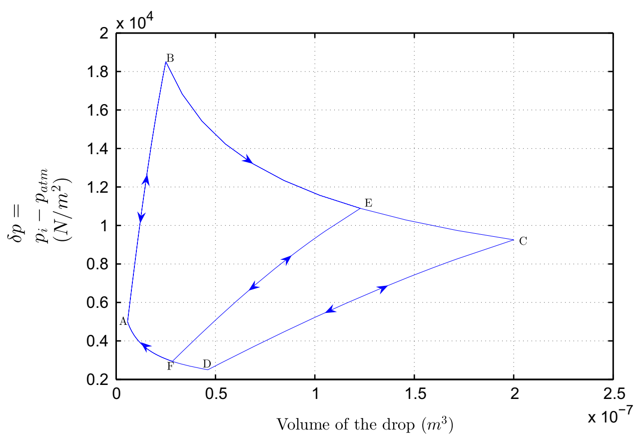

Fig. 2. Hysteresis curves for a liquid drop with $R = 0.02$ m. δp indicates the pressure difference between the liquid–gas interface of a liquid drop. Points B and C correspond to the advancing ($\theta_a = 40^\circ$) and receding ($\theta_d = 10^\circ$) contact angles of the droplet.

2. Model formulation for capillary surface

To make the problem amenable to analysis, we consider a simplified problem where a liquid and a gas are bounded between two parallel plane walls with a capillary surface between the liquid–gas interface. The relative importance of the phenomena causing dissipation of energy may be determined by analyzing this system.

Using calculus of variations, we obtain the mathematical model for a capillary surface at equilibrium, by minimizing the total energy subject to a constant volume constraint [2–4]. In Ref. [3], the author considers a liquid drop between two vertical plates, and neglects the potential energy due gravity. The presence of gravity makes the problem significantly different as it causes a pressure change with depth in the fluid – mathematically, Eqs. (2) and (3) form a two point boundary value problem which is well-posed due to the fact that $g \neq 0$.

In our analysis, we consider a liquid meniscus that formed between two vertical plates, and assume the invariance of the liquid surface in the z-direction (see Fig. 1(a)), which effectively makes the problem a two-dimensional one, and the walls to be hydrophilic. Furthermore, the potential energy due to the gravitation is also included in our total energy functional. The capillary surface $f(x)$ defined over the interval $[0, L]$ satisfies a second-order ordinary differential equation (1). Specification of the contact angles at the two walls (θ_1 and θ_2), which are related to $f'(0)$ and $f'(L)$, yields a two point boundary value problem that we solve numerically using the modified simple shooting method [5]. The height of the capillary surface $f(x)$ is specified with respect to the depth where the liquid pressure equals the atmospheric pressure.

Consider two plates of unit-width as in Fig. 3(a). The $x-z$ plane corresponds to the depth where the pressure in the liquid is equal to the atmospheric pressure. Let the liquid volume between the $x-z$ plane and under the capillary surface be V_0. Let ρ denote the density of the liquid, γ denote its surface tension coefficient, β_1, β_2 denote the relative adhesion coefficients for the two walls, and g denotes the magnitude of gravitational acceleration. The necessary condition for the energy minimization [4] lead to the following systems:

$$\rho g f(x) - \gamma \frac{f''(x)}{\sqrt{(1+f'^2(x))^3}} + \lambda = 0 \quad \text{in } [0, L], \tag{1}$$

$$\int_0^L f(x)\, dx = V_0 \tag{2}$$

$$\beta_1 + \frac{f'(0)}{\sqrt{1+f'^2(0)}} = 0; \qquad \frac{f'(L)}{\sqrt{1+f'^2(L)}} - \beta_2 = 0. \tag{3}$$

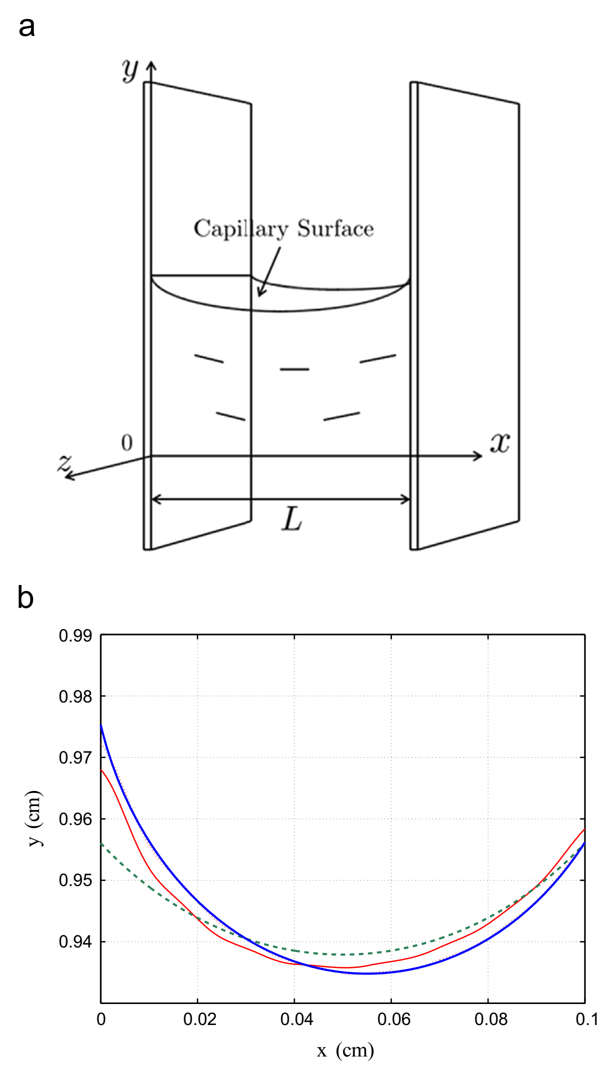

Fig. 3. (a) The y-axis is placed along the vertical plate, and the x-axis is perpendicular to the plates. Gravitational acceleration **g**, acts along the $-y$ direction. (b) Initial (dashed) and final (solid-bold) capillary surface profiles. The intermediate curves (solid-thin) are computed by solving a two-point boundary value problem for the Navier–Stokes and continuity equations for $N = 10$ and $\varepsilon = 5000$.

The Lagrange multiplier λ may be calculated by integrating Eq. (1) and using $f_x(0) = -\cot\theta_1$, $f_x(L) = \cot\theta_2$, where θ_1 and θ_2 denote the contact angles between the liquid meniscus and the plates 1 and 2, respectively. Hence, one can relate the value of β_i that is given in the constraint equation (3) with the corresponding contact angle θ_i, which yields to

$$\beta_1 = \cos\theta_1; \quad \beta_2 = \cos\theta_2. \tag{4}$$

First, we obtain the initial capillary surface ($y_i(x)$) by solving (1) with $\lambda = 0$ together with the boundary conditions: $f'(0) = -\cot\theta_1$ and $f'(L) = \cot\theta_2$. We calculate the corresponding liquid volume V_0 using Eq. (2), and it serves as the constraint on the volume for the subsequent deformations of the initial surface. The second surface ($y_f(x)$) is numerically obtained by solving (1) and (2) with the boundary conditions: $f(0)$ and $f(L)$, where $f(L) = y_i(L)$. Due to the contact angle hysteresis phenomenon [1], the initial and final capillary surfaces have different contact angle values (and heights) at the walls 1 and 2.

3. Analysis of the fluid flow leading to deformation of the capillary surface

In this section, we solve for the initial velocity field of the liquid that takes an initial capillary surface $y_i(\cdot)$ to a final one $y_f(\cdot)$ while obeying the Navier–Stokes and continuity equations. We consider a Newtonian, incompressible fluid, with dynamic viscosity μ, and velocity $\mathbf{u} = (u(x,y,t), v(x,y,t))$. As the liquid has zero velocity in the x direction at $x=0$ and $x=L$, a choice $u(x,y,t) = u_0(t)\sin(\pi x/L)$ leads to one class of solutions.

From the x-component of the N–S equation [6], we have both $u_0(t) = e^{-\mu/\rho(\pi^2/L^2)t}u_0$ and $(\rho/2)u_0^2(t)\sin(2\pi x/L)\pi/L = -\partial p/\partial x$. Therefore, the pressure inside the fluid is $p(x,y,t) = (\rho/4)u_0^2(t)\cos(2\pi x/L) + \overline{p}(y,t)$. The continuity equation [6] yields

$$v(x,y,t) = A(x,t) - \frac{\pi}{L}u_0(t)\cos\left(\frac{\pi x}{L}\right)\int_0^y \phi(s)\,ds,$$

for some function ϕ. The choice $\phi(s) = 1$ yields one solution. Next, we apply techniques of Fourier analysis to the y-component of the N–S equation. Assume that $A(x,t)$ is given by

$$A(x,t) = \frac{\alpha_0(t)}{2} + \sum_{k=1}^{\infty}\alpha_k(t)\cos\left(\frac{k\pi x}{L}\right) \tag{5}$$

over the interval $[-L, L]$, where for each t, it is also assumed that $A(x,t) = A(-x,t)$. We substitute in the series for $A(x,t)$ into the y component of the N–S equation and equate terms on each side for each k. For $k=0$, we have

$$\frac{\alpha_0'(t)}{2} - \frac{\pi}{L}u_0(t)\alpha_1(t) + \frac{\pi^2}{L^2}u_0^2(t)y = -g - \frac{1}{\rho}\frac{\partial\overline{p}}{\partial y}. \tag{6}$$

If, for some function ξ, the functions α_0, α_1, u_0, and $\overline{p}$ satisfy $\alpha_0'(t)/2 - (\pi/L)u_0(t)\alpha_1(t) = \xi(t)$ and $(\pi^2 L^2)u_0^2(t)y + g + 1/\rho\ \partial\overline{p}/\partial y = -\xi(t)$ then they automatically satisfy (6). Thus, different choices of ξ lead to different solutions. We choose $\xi(t) = -\varepsilon\alpha_0(t)$ for $\varepsilon > 0$, as otherwise the y-component of the N–S equations lead to an unstable system.

Consider the boundary value problem defined by the initial and the final capillary surfaces $y_i(x)$ and $y_f(x)$, and suppose $y_f(x) - y_i(x) = a_0/2 + \sum_{k=1}^{N} a_k\cos(k\pi x/L)$. By using the kinematic free surface boundary condition, the meniscus profile at time t, that is $y(x,t)$, may be expressed using

$$y(x,t) = y_i(x) + \int_0^t \left(v(x, y(x,s), s) - \frac{\partial y(x,s)}{\partial x}u(x,s)\right) ds$$

Table 1
Viscous energy dissipation and initial kinetic energy variations with different ε values.

N	ε	$D \times 10^{-4}$ (erg)	KE^{ini} (erg)
10	5000	3.64	0.0210
	7000	3.54	0.0201

which yields

$$y_f(x) = y_i(x) + \int_0^{\infty}\left(v(x, y(x,t), t) - \frac{\partial y(x,t)}{\partial x}u(x,t)\right) dt. \tag{7}$$

By using the series expansions of $v(x,y,t)$ and $y_f(x) - y_i(x)$, we rewrite Eq. (7) in the following form:

$$\frac{a_0}{2} + \sum_{k=1}^{N} a_k\cos\left(\frac{k\pi x}{L}\right) = -\left(\frac{c_0}{2} + \sum_{k=1}^{N} c_k\cos\left(\frac{k\pi x}{L}\right)\right) + \int_0^{\infty}\frac{\alpha_0(t)}{2} + \sum_{k=1}^{N}\alpha_k(t)\cos\left(\frac{k\pi x}{L}\right)dt,$$

where we assume that the term: $\int_0^{\infty}(\pi/L\,\cos(\pi x/L)y(x,t)u_0(t) + \partial y(x,t)/\partial x u(x,t))\,dt$ has the Fourier series $c_0/2 + \sum_{k=1}^{N} c_k \cos(k\pi x/L)$. Then, the resulting system of equations is solved together using a modified simple shooting method [5] to obtain $\alpha_k(t)$, $k \geq 0$.

4. Numerical results and discussion

The non-uniqueness in the solutions are due to (a) choice of the form for $u(x,y,t)$, (b) choice of the form for $v(x,y,t)$, and (c) choice of $\xi(t)$. The first two reasons lead to *theoretically* non-unique solutions. Even after the form of u and v are fixed, the last reason leads to non-uniqueness in numerically computed solutions. This is because no matter what ξ is, Eq. (6) is always satisfied. However, the choice of ξ can yield numerically different solutions unless one is careful in selecting ε and the number of modes N for a solution. For discretization parameters δt and δx for time and the spatial coordinate respectively, we select $N \leq L/10\delta x$ and $5N^2\eta \leq \varepsilon \leq -\ln(0.5)/\delta t$. For $\delta t = 10^{-4}$ and $\delta x = 10^{-3}$, the choice of N and two different ε values shown in the table (Table 1) above show similar results. It must be noted that for a choice of $\varepsilon = 2000$ and $N = 10$, which does not satisfy the inequalities presented above, we found the kinetic energy to be $KE = 0.0075$ ergs, and the energy dissipated due to viscosity to be $D = 2.21 \times 10^{-4}$ ergs. This shows that there exist numerically non-unique solutions depending on the choice of ξ.

The numerical results are shown in Fig. 3(b). Other numerical solutions corresponding to different choices of u and v needs to be done in the future.

5. Conclusions

In this paper, we investigated the dynamic motion of a capillary surface that forms between two vertical plates. We considered the Navier–Stokes and continuity equations to set up a two-point boundary value problem for fluid motion that deforms the capillary surface. We showed that there exist non-unique solutions to the problem.

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