Migration of droplets driven by thermocapillary effects

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Se estudia el desplazamiento de gotas, en dos dimensiones y bajo condiciones de mojabilidad parcial, ubicadas sobre un sustrato calentado en forma no uniforme. Se resuelve la ecuación que gobierna el perfil de altura de la gota, bajo las hipótesis de lubricación. El modelado incluye el efecto de la mojabilidad parcial (ángulo de contacto no nulo) mediante un término que representa las fuerzas intermoleculares entre el sustrato y el líquido. En vez de asumir una forma fija para la forma de la gota, como en trabajos previos, aquí se resuelve la evolución temporal del perfil de altura. Hemos identificado dos regímenes de flujo y una zona de transición.

Palabras Claves: gotas, termocapilaridad, mojamiento parcial.

We study the thermocapillary migration of two dimensional droplets of partially wetting liquids on a non-uniform heated substrate. An equation for the thickness profile of the droplet is solved under the hypothesis of the lubrication theory. The model includes the effect of a non-zero contact angle introduced through a disjoining-conjoining pressure term. Instead of assuming a fixed shape for the droplet, as in previous works, here we allow the droplet to change its profile with time. We identify and describe two different regimes and a transition zone.

Key Words: droplets, thermocapillarity, partial wetting.

I. INTRODUCTION

In this article we focus our attention on the thermocapillary actuation of liquids on horizontal surfaces. The movement of the fluid is achieved by imposing a temperature gradient on the substrate that produces a temperature gradient at the liquid-air surface. This non-uniformly heated interface induces a surface tension gradient which exerts a hydrodynamic force that moves the droplet from warmer to colder regions.

Experiments performed under partial wetting conditions (non zero contact angle) have shown that the droplets move with a constant velocity and keep a fixed shape [1–3]. The theoretical study of this problem is usually simplified to the study of a two dimensional droplet under the influence of a shear stress at the liquid-air interface, the flow being solved within the lubrication theory. In accordance with experiments, the authors solve the problem under stationary conditions [4, 5].

Marangoni wetting films climbing a plate against gravity by thermally induced surface tension gradients constitutes another example of thermocapillary actuation of fluid [6, 7]. The main difference between this and the constant-volume droplet problem is that in Marangoni films there is a continuous pumping of fluid from a container towards the advancing front. The typical profile is characterized by a long film connecting the fluid in the container with a capillary ridge formed at the leading edge. Ludviksson & Lightfoot (1971) studied the evolution of these films and found that the substrate is coated at a constant rate. As we shall see, these Marangoni film type profiles will be relevant to the drop migration problem in certain parameter ranges.

The analysis of these experiments can lead one to falsely conclude that the only difference between the dynamics of

droplet and Marangoni films flows is the different experimental conditions (the former conserves the mass while the latter does not). However the fact that the experiments in Marangoni film flows are performed using wetting fluids while the actuation of droplets is typically carried out for partially wetting liquids suggests that wettability may play an important role. In order to examine this point, we present results on the study of the effect of non-zero contact angle (partial wettability) on the thermocapillary actuation of droplets. In particular, we discover important differences in flows with low and high contact angle. An improvement on previous theoretical analysis is that here, instead of considering a droplet moving with a constant velocity and a steady shape as usually assumed, we solve an initial value problem for the thickness h and motion of the droplet, imposing restrictions neither on the velocity of both the contact lines and the drop nor on the drop shape.

II. MODELLING

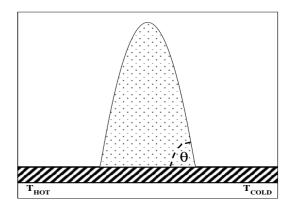


FIG. 1: Static droplet in contact with a flat molecular film.

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Consider a two dimensional droplet deposited on a horizontal substrate which is subject to a constant temperature gradient, as shown in Fig. 1. We define the dimensionless variables $\hat{x} = x/a$, $\hat{h} = h/a$ and $\hat{t} = t/t_c$ with $t_c = 3\mu a/\gamma$, where $a = \sqrt{\gamma/\rho g}$ is the capillary length, μ is the viscosity, ρ is the density and g is the gravity. Assuming (a) small Biot and Peclet numbers [2] and (b) a linear dependence between the surface tension γ and the temperature T, the standard dimensionless equation for the thicknnes h is [8]

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \left(h^3 \frac{\partial^3 h}{\partial x^3} \right) + B \frac{\partial h^2}{\partial x} +$$

$$K \frac{\partial}{\partial x} \left(h^3 \frac{\partial}{\partial x} \left[\left(\frac{h_*}{h} \right)^3 - \left(\frac{h_*}{h} \right)^2 \right] \right) = 0.$$
(1)

The last term is the disjoining-conjoining pressure that accounts for the intermolecular forces between the solid and the liquid. The constant K, a measure of the contact angle θ , and B, a Marangoni number, are defined as

$$K = \frac{2(1 - \cos \theta)}{h_*},$$

$$B = \frac{3a\tau}{2\gamma_0}.$$
 (2)

Here h_* is the thickness of the energetically favoured molecular film in units of a and $\tau = (d\gamma/dT)(dT/dx)[9]$.

We discretize Eq. (1) in space using regular centred finite differences and the resulting system of equations are evolved in time by employing a synchronized marching Crank-Nicholson scheme combined with an adaptive time stepping procedure (details about the numerical method can be found in Ref. [10]). The initial condition corresponds to the case B=0.

III. FILM REGIME: SMALL CONTACT ANGLE

In this regime the droplet increases its width and, after a transient stage, the bulk region exhibits a linear profile, as shown in Fig. 2. Here, the contact angle is small and thus the effect of the disjoining-conjoining pressure term is negligible. The numerical solution shows that the curvature in the bulk region is small and therefore the effect of the capillary pressure term is also negligible. Neglecting both terms, the behaviour away from the leading and trailing edges can be captured by a simple self-similar solution:

$$h = \frac{x}{2Bt} \quad \text{for} \quad x_R \le x \le x_L, \tag{3}$$

 x_R and x_L being the position for the rear and leading fronts:

$$x_R = x_0 + 2h_{film}Bt$$

$$x_L = x_R + \sqrt{4ABt}.$$
(4)

Experiments carried out for Marangoni films of wetting liquids have shown, at least in one case, a linear profile connecting the advancing ridge with the fluid in the container [11].

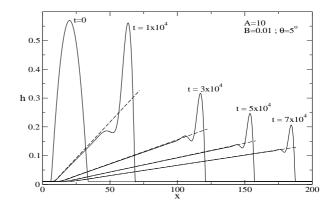


FIG. 2: Evolution of the thickness profile obtained by solving 1 (solid lines) and the asymptotic profiles given by 3 (dashed lines). The profiles correspond to the case with $\theta = 5^{\circ}$, A = 10, B = 0.01 and $h_* = 0.01$.

IV. DROPLET REGIME: LARGE CONTACT ANGLE

Contrary to what we observed for small contact angles, here the droplet moves keeping its original steady shape as shown in Fig. 3(a). Hence we refer to this as the Droplet Regime. In this range of parameters, the effect of the disjoining-conjoining pressure is stronger than in the previous case and the Marangoni stress induced at the liquid-air interface cannot change the shape of the droplet. Interestingly, the inspection of the region close to the substrate shows that the while the droplet advances the rear front leaves a constant thickness thin film, as depicted in Fig. 3(b). The height of this film decreases when either θ or A is increased. The numerical simulations

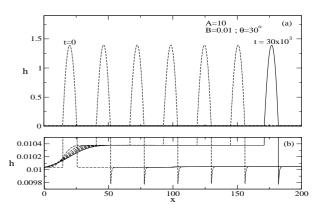


FIG. 3: Evolution of the droplet profile with $\theta=30^\circ$, A=10, B=0.01 and $h_*=0.01$. (a): Quasisteady droplet motion shown at equal time intervals. The solid line is the last profile for $t=30\times10^3$. (b): A zoom of the region close to the substrate.

show that the velocity of the droplet is proportional to B, in agreement with experimental results [1].

Before presenting the regime maps, it is worth to mention that for intermediate values of θ we have observed that the Marangoni and disjoining-conjoining pressure terms compete and thus the dynamics of the flow is complex: preliminary results show breakup processes that would require an exten-

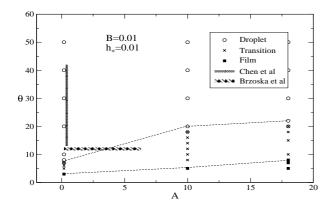


FIG. 4: Map of the Film, Droplet and Transition regimes in the θ - A space. The experimental data corresponds to the experiments reported in [1] and [2]. Note that in Brozska's experiments $0.002 \le B \le 0.007$, i.e. a value of B lower than that of these simulations.

sive parametric study in order to be analysed. With the aim of study the occurrence of the Marangoni and Droplet regimes, in what follows we refer to this complex dynamics as the Transition regime and the detailed study of this complex dynamics is left for future work.

V. REGIME MAPS

Here we study how the parameters A and B affect which regime may occur. We do this by representing the different regimes in the θ - A plane, with B as a parameter. Figure 4 shows one of these maps for B=0.01. Notice that the two regimes - Film and Droplet - can be observed for the range of A studied. Interestingly, due to the fact that the integral effect of the disjoining pressure on the whole volume is more important for smaller droplets than for larger ones, the values of θ at which we observe the transition from Film to Transition regimes and from Transition to Droplet regimes are lower for the smaller values of A. For example, for A=0.18, the values of the contact angles define the boundary between the Film-Transition and Transition-Droplet regimes are $\theta_{FT}\approx 5^\circ$ and $\theta_{TD}\approx 7^\circ$, respectively, while the corresponding contact angles for A=18 are $\theta_{FT}\approx 9^\circ$ and $\theta_{TD}\approx 20^\circ$.

These diagrams help explain why the Droplet regime is the only one reported to date when a constant volume is considered. In the experiments of [2], $B \approx 0.01$, $A \approx 0.37$, all cases fall within the Droplet regime: thus the experiments are in agreement with our results with regard to the regime that occurs. Figure 4 suggest that the highest values of A in experiments of [1] fall in the Transition regime, but those experiments were performed with smaller values of B: the more relevant comparison is with Fig. 5.

Figure 5 (a,b) presents the same diagram but for B = 0.05 and B = 0.002, respectively. We can observe that when the value of B is decreased (increased) the contact angles θ_{FT} and θ_{TD} reduce (increase) their values. The results for B = 0.002 bring the theory and the experiments of [1] into better agreement: the Film Regime disappears for small values of A as

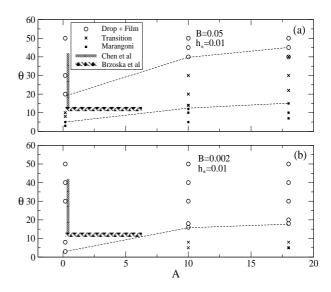


FIG. 5: Effect of *B* in the distribution of the flow regimes on the θ -*A* plane.

reported in experiments, a result that is consistent with those experiments (for which $0.002 \le B \le 0.007$), all of them falling in the Droplet regime.

VI. CONCLUSIONS

We have considered the thermocapillary migration of droplets on horizontal surfaces. We employed lubrication theory to derive an equation for the droplet profile that includes the effect of the disjoining-conjoining pressure. The form of the chosen disjoining-conjoining pressure term admits a nonzero contact angle at the contact line region. One of the main differences with previous works is that we do not assume a constant spreading velocity, but rather we allow the droplet to evolve its shape in time.

We report two different flow regimes. We find that for small contact angles the droplet continuously increases its width. The droplet adopts a linear shape in an outer region, a profile captured by a self similar solution. For large θ , the droplet approximately keeps its steady initial shape. A thin film is left behind the rear front. For intermediate values of θ we observe a Transition Regime in which the dynamics is complicated and its study is left for future work.

The occurrence of these regimes is very sensitive to the values of A and B. We display our results in a map in the θ - A plane and find that, for a given B, the limiting contact angle that separates the Film-Transition and Transition-Droplet regimes are smaller for smaller A. Employing the same diagram, but for a lower value of B, we observe that these limiting contact angles decrease, and the Film Regime does not occur even for the smallest contact angle analysed. For large B, the limits move toward higher values of θ . In spite of the relative simplicity of the model, all these trends are in agreement with available experiments.

Acknowledgements

This work was supported by the US DOE through grant number DE-FG02-05ER15692. JMG gratefully acknowl-

edges the Fulbright Foundation and CONICET for partial support.

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