Contact Lines on Rough Surfaces with Application to Air Entrainment*

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Introduction

A simple explanation for moving contact lines based on surface irregularities has been proposed by L.M. Hocking[1]. His thesis is that fluid slip at a solid boundary cannot occur at microscopic scales, but surface irregularities with microscopic scales can induce flow structures that may be interpreted as slip from a macroscopic point of view. In this paper we use computational fluid dynamics simulations to show in detail how a contact line can move over rough surfaces.

At a liquid/air interface moving over a solid surface there should be no velocity slip. However, it is well known [2,3] that flow at a contact line, when modeled using a continuum description, exhibits singularities. The singularities are associated with the use of continuum flow equations (i.e., the Navier-Stokes equations) together with the no-slip boundary condition [3]. Having said this, it is important to recognize that this difficulty with singularities is confined to a region about the contact line of molecular scale where there is no reason to expect a continuum model to be valid.

In this paper we use a finite-control-volume technique, which does not require the introduction of ad hoc assumptions. The finite-control-volume method simply keeps track of the mass, momentum, and energy in the control volume element. The locations of contact lines and the location of fluid surfaces or interfaces are tracked by a volume-of-fluid (VOF) method in which the fraction of liquid in each computational grid element is recorded. With the fluid fraction value in an element together with the fractional values in neighboring elements one can easily locate surfaces and even compute surface slopes and curvatures [4].

At a contact line the only additional consideration needed beyond the standard dynamic processes contained in the Navier-Stokes equations is a mechanism to describe the adhesion between liquid and a solid substrate. This is done by assuming that the adhesion force, which arises from molecular interactions between solid and liquid, can be characterized by a static contact angle. In any grid element containing a contact line (i.e., a fluid interface and a solid surface) an additional adhesion force is computed and added to the other forces acting on the element (e.g., pressures, body forces, viscous stresses, advective processes, etc.). The additional force is computed from the slope of the fluid surface with respect to the solid surface and assuming that Young's equation describes the proper balance of forces under static conditions [5].

In dynamic situations involving moving contact lines, we continue to compute adhesion forces using the static contact angle, a physical quantity that can be easily measured. This is justified because the molecular processes responsible for adhesion forces occur on space and time scales that are orders of magnitude smaller and faster, respectively, than those of macroscopic flow processes. Because of this, the macroscopic processes cannot have any significant influence on the molecular level.

Dynamic contact angles are not specified but computed as part of the solution in the finite-control-volume method based on the VOF technique. They arise automatically from the balance of forces in the vicinity of the contact line. This is one of the several practical advantages of this modeling approach.

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All the simulations presented in this paper were performed using this combined control-volume-VOF approach as it has been implemented in the commercial software program ***FLOW-3D®*** developed by Flow Science, Inc. located in Santa Fe, New Mexico, USA. Reference [6] may be consulted for additional information about this program.

In the remainder of this paper we shall look into the issue of microscopic roughness and show how it can change dynamic contact angles, approximate slip conditions, and what effect web roughness may have on air entrainment at the upstream contact line in slot coating.

Flow over a Rough Surface

L.M. Hocking has proposed [1] that contact lines move over a solid surface because microscopic irregularities induce flow structures that may be interpreted as “velocity slip” from a macroscopic point of view. To test this proposal computationally we shall study the passage of a contact line over a rough surface consisting of transverse, regularly spaced, rectangular slots. For our test case the slots are 2μm deep and 10μm wide, and spaced to have 10μm wide solid pieces between them. These dimensions are typical of roughness features on medium-ground steel surfaces. The static contact angle with the solid was chosen to be 120°. Water is the working fluid. The test consisted of driving water at 30cm/s through a two-dimensional channel of height 15μm, having a free-slip top boundary.

In the first test, used as a control, the “roughness” slots along the bottom of the channel were omitted. The contact line moves smoothly over the solid surface, Fig.1a, with a dynamic contact angle equal to the static contact angle of 120°. Because of the small capillary number in this example, Ca=0.004, this result was expected.

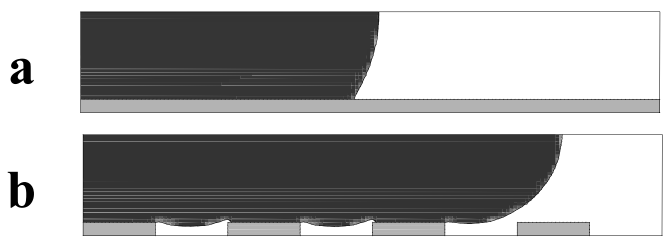

Figure 1. Flow of liquid with static contact angle 120° over (a) smooth surface and (b) a rough surface.

Repeating the simulation with the rough boundary, it is immediately evident that the water surface gets attached to the edge of a slot and remains there until the surface becomes nearly horizontal and makes contact with the next, downstream portion of the boundary, Fig.1b. The liquid cannot fill in the slots because of the contact angle on the vertical side of the slot never exceeds the static contact angle. An effective, advancing contact angle for this case is a mixture of the 120° angle when the contact line moves across the solid portions of the boundary and 180° while the liquid surface is pulled out flat from the edges of the slots. If β is the fractional area, per unit area, of solid surface then the effective advancing contact angle θ_a is approximated by $\theta_a=120\beta+180(1-\beta)$. This result is basically the same as that found for flow over fabric surfaces, which consist of parallel rows of circular cylinders instead of rectangles [7].

Hocking’s assertion that micro-scale disturbances can be interpreted as a kind of velocity slip when looked at over larger scales is supported by the computed velocity field. This is shown graphically in Fig.2, which gives the horizontal velocity distribution in the layer of control volumes immediately above the surface. With further grid refinement, the velocity above the solid portions of the surface would tend to zero, but above the slots the velocity remains non-zero. A macroscopic view that averages the flow over many roughness elements would see a non-zero horizontal velocity that could be interpreted as an effective slip.

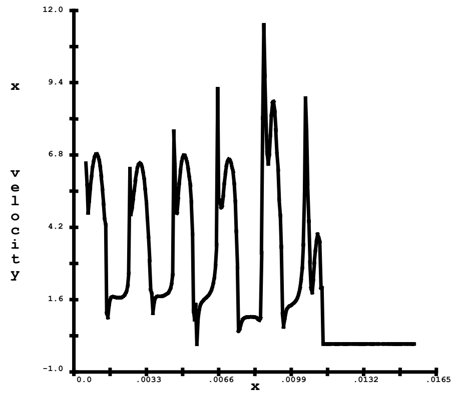

Figure 2. Horizontal velocity profile immediately above solid surface.
Horizontal line segment at right side is zero velocity level.

Air Entrainment

The ability to model the transient behavior of a contact line makes it possible to investigate a variety of mechanisms that could lead to the entrainment of air at a contact line. For instance, one possibility is that small irregularities on the surface of a web could cause perturbations large enough to cause the liquid to temporarily leave the surface and trap some air. A simple test with water and 2μm high dip and bump perturbations shows that at small capillary numbers (e.g., 0.04 in the present case) surface tension forces are so strong that the contact line easily rides over the perturbations and cannot be detached from the web surface. The static contact angle used for these simulations was 30°.

However, if a perturbation has a non-wetting surface (e.g., because of some contamination) then it is possible for small amounts of air to be entrained. This is shown in Fig. 3 where the right perturbation in each case has a non-wetting surface (i.e., static contact angle of 140°). Both the bump and dip perturbations with non-wetting surfaces entrain air because the contact line is not able to flow over them.

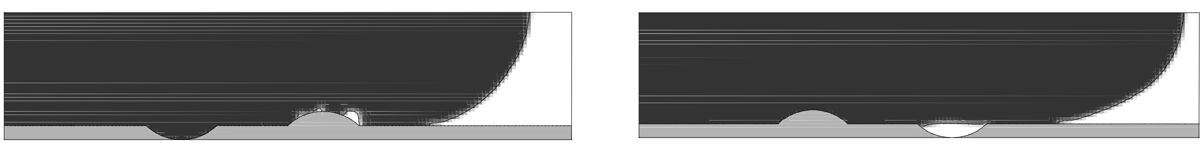

Figure 3. Air entrainment at non-wetting bump and dip perturbations.

Conventional wisdom is that air entrainment at a contact line does not occur until the dynamic contact line reaches a value of 180°[8]. For this to happen the capillary number must be relatively large, i.e., viscous forces must dominate those of surface tension. Figure 4 shows this transition in dynamic contact angle when the test case (web speed 3m/s) is repeated with a successively larger viscosity assigned to the liquid. The dynamic contact angle is computed to increase from the 30° static value at Ca=0.04 to near 180° at Ca=4.0.

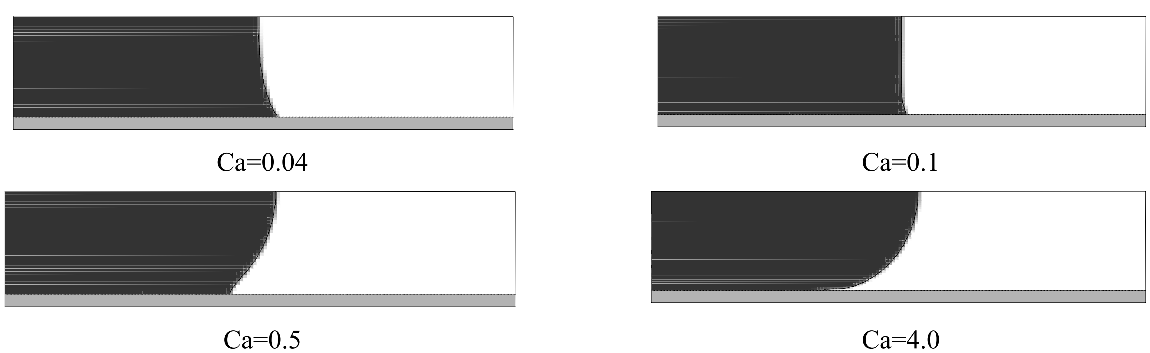

Figure 4. Dynamic contact angle computed as function of capillary number.

Summary

A numerical simulation method has been used to investigate the microscopic behavior of a moving contact line in the presence of roughness elements. The qualitative, macroscopic results agree with observations, but the details of the local flow behavior, which has never been directly observed, is found to be quite complex. The results presented support the hypothesis made by Hocking[1] for the motion of a contact line over a solid surface.

Preliminary results have been presented for possible mechanisms leading to air entrainment at a contact line. This work shows how a modeling approach based on the application of basic conservation principles applied to small control elements can be exploited to study the dynamic behavior of contact lines.

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