FSI-99-00-2

DIRECT COMPUTATION OF DYNAMIC CONTACT ANGLES AND CONTACT LINES

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Presented at ECC99 Coating Conf., Sept. 1999, Erlangen, Germany

SUMMARY

The location of dynamic contact lines and the determination of dynamic contact angles are important for the understanding and prediction of many types of coating flow processes. Dynamic contact angles are a result of all the forces acting on a fluid; for example, viscous, gravitational, surface tension, wall adhesion, inertia and air pressure forces. Because dynamic contact angles develop in response to a local balance of forces, they are not an intrinsic fluid property. This fact is a source of difficulty for many numerical techniques, especially those that must locate a node or data point precisely at a contact line location. In these methods it is often necessary to use a slip boundary condition or to introduce additional physical phenomena such van der Waal's forces or thin precursor films to have well-defined boundary conditions.

In this presentation we describe a computational method that allows for the direct computation of contact lines and dynamic contact angles from basic fluid dynamic principles. This technique uses a fixed grid of control volumes and a Volume-of-Fluid (VOF) method to compute the average flow conditions in the vicinity of contact lines. The location and slope of a fluid interface at a contact line are not specified but are automatically evaluated as part of the solution process.

1. BACKGROUND

The line of intersection between a liquid surface and a solid surface is called a contact line. Molecular interactions between liquid and solid constituents along a contact line can lead to a net force of attraction (wetting) or repulsion (non-wetting) between the liquid and solid. The angle between the liquid surface and the solid surface is called the contact angle.

For many applications the contact line is stationary with respect to the solid and the corresponding "static" contact angle has a unique value that depends only on the liquid and solid materials. A more interesting case develops when the liquid is moving with respect to the solid. For example, when you see a raindrop running down the side window of a car the contact angle at the leading edge is larger than that at the trailing edge. These "dynamic" contact angles depend on the forces acting on the fluid: viscous, gravitational, surface tension, wall adhesion, and air pressure.

Because the dynamic contact angle is a resultant of several forces, and may even be time-dependent if there are changes occurring in those forces, it is not a property of the fluid. For this reason the dynamic contact angle cannot be specified and becomes a source of difficulty for many numerical techniques used to compute flows involving contact lines (e.g., coating flows). The difficulty is associated with a desire (or need) to specify flow conditions precisely at the contact line.

The motion of liquid in a capillary tube illustrates the difficulty. Imagine the interface between two fluids inside of a capillary tube that is moving at a fixed speed with respect to the wall of the tube. A pressure difference applied to the ends of the tube may be required to maintain the constant speed of the interface. A contact line exists where the two-fluid interface intersects the tube wall, Fig. 1. At the contact line there arises a paradox: how can the fluid interface move along the wall of the tube and at the same time satisfy a no-slip boundary condition on the wall?

To apply a finite-element numerical method to this problem it is natural to locate a node point at the contact line since this point is on the boundary of the fluid. Unfortunately, this is a poor choice because flow conditions are not well defined at the contact line. To get around this difficulty many researchers have introduced ad hoc assumptions. For instance, it is popular to introduce slip on the solid surface in the neighborhood of the contact line[1], or to add new physical phenomena (e.g., van der Waals forces and thin precursor films) in an attempt to get a mathematically consistent model at the contact line[2].

In the next section we briefly consider the practical aspects of modeling contact lines. This is followed by a description of a computational approach that directly computes contact lines and dynamic contact angles from basic fluid dynamic principles.

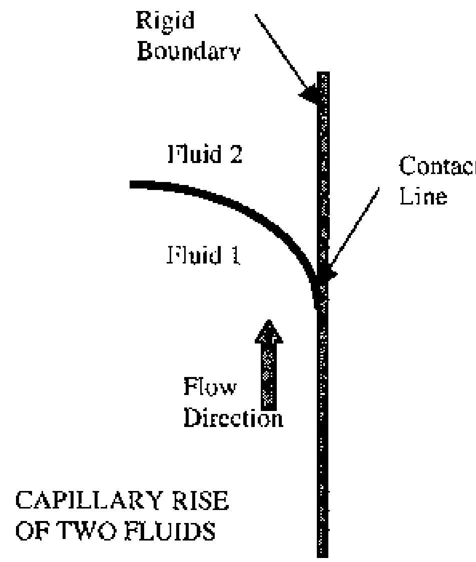

Figure 1. Contact line problem.

2. PRACTICAL CONSIDERATIONS AT CONTACT LINES

From a continuum point of view, the requirement of a no-slip boundary condition at a solid surface is inconsistent with a moving contact line. To gain a better appreciation of what happens at such a point it is useful to review the results of molecular dynamics simulations.

A paper that explicitly considers the problem of a two-fluid interface adjacent to a moving solid boundary is that by Thompson and Robbins[3]. In this paper the authors show that the no-slip condition on the solid boundary is valid everywhere, except for distances on the order of a couple of molecular diameters in the vicinity of the contact line. This makes physical sense, because molecules hitting the boundary clearly experience its effect but cannot sense other boundary effects when they are more than a few molecular diameters distant.

From this point of view, no-slip wall conditions must hold at distances beyond about 10^{-9}m. The minimum distance that can be observed in laboratory experiments is on the order of 10^{-6}m or larger, so the minimum observable feature is three orders of magnitude bigger than the size over which wall slip could occur. Therefore, it makes little sense, from a practical point of view, to introduce a wall-slip condition in the vicinity of a contact line.

3. THE VOLUME-OF-FLUID (VOF) METHOD FOR CONTACT LINES

Let a flow region be subdivided into a fixed grid of rectangular cells. The specification "fixed" means that liquid will be allowed to flow through this (Eulerian) grid. To locate liquid surfaces in the grid a volume-fraction or Volume-of-Fluid (VOF) function, F, is used where F is the fraction of a grid element that is occupied by liquid. An element filled with liquid (F=1) must be in the liquid interior, while an empty element (F=0) is outside the liquid. Liquid surfaces are located in elements that are partially filled.

The function F can also be used to compute the slope and curvature of a surface. To do this it is necessary to assume that F is a step function that passes discontinuously between values of zero and one at a surface.

The VOF method may be used with a finite-volume numerical solution technique for the Navier-Stokes equations. The key is to use the proper free-surface boundary conditions (i.e., normal and tangential stress conditions) in elements containing a fluid surface. Examples of this numerical approach can be found in Ref. 4 and more extensively on the Internet at www.flow3d.com.

For present purposes it is only necessary to review why this numerical approach is useful for the treatment of contact lines. Consider the two-dimensional grid elements shown in Fig.2, which contain a free surface and a solid boundary along the left side. The restriction to two dimensions

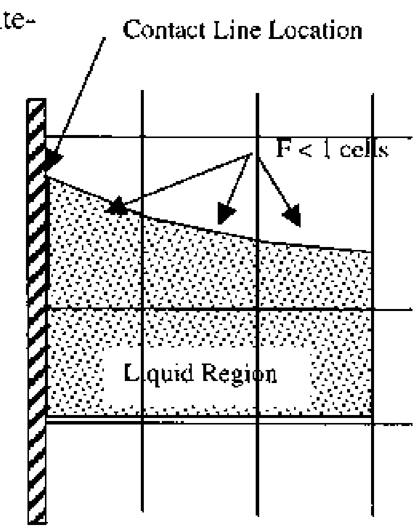

Figure 2. A VOF fixed grid with partially filled cells (fluid fractions less than one) that define the liquid surface.

is only for presentation purposes, the technique applies equally as well to three-dimensional situations.

The location where the liquid surface intersects the solid (the contact line) is not specified, it moves up or down with a grain or loss of liquid in the cell.

That is, if a sufficient amount of liquid enters the cell containing the contact line it will move upwards into the cell above. With a loss of liquid it moves downward.

Liquid velocity components are located at the faces of the elements, as shown in Fig.3. This placement is ideal for computing the volume of liquid that passes between elements. These components represent the average velocity of liquid in their vicinity and are not associated with a particular point such as a contact line.

The velocity components computed in the element containing the contact line depend on all the forces acting on the liquid in this element. These include a shear stress at the solid wall, viscous stresses arising from velocity gradients with neighboring elements, adhesion on the wall, pressures acting on the element (both exterior gas as well as interior liquid pressures), surface tension, and gravity.

Since neighboring elements have flows computed in a similar way, the net result is that the location of the contact line and its slope are determined automatically from the computations. Although only "average" properties are being computed for each element, the size of the elements can be made as small as one likes.

4. DYNAMIC CONTACT LINE EXAMPLE

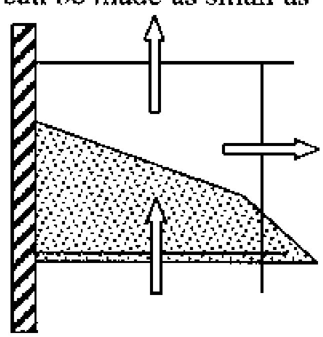

Figure 3. Location of velocity components in an element.

A plunging-tape example studied with the VOF technique has been previously reported[5]. Here we concentrate on an example of capillary-rise in a tube. For simplicity, and comparison with previous work, we consider the interface between two fluids having the same density and viscosity. The fluid interface is moving uniformly up a vertical capillary tube of circular cross section. A pressure gradient is applied along the length of the tube to maintain a constant interfacial speed. In non-dimensional terms, the problem has Capillary number $Ca=\mu U/\sigma=0.01$ and Reynolds number $Re=\rho UR/\mu=0.05$.

For modeling purposes it is better to be in a frame of reference that is stationary with respect to the interface. This is accomplished by translating the tube wall downward at the same speed the interface is moving upward. Surface tension acts at the interface and a static contact angle of 100° has been assumed at the tube wall. The choice of a non-wetting, static contact angle was arbitrary; its principal effect is to alter the magnitude of the axial pressure gradient needed for steady flow conditions.

An example of previous modeling done on this class of problems is the work of Sheng and Zhou[6], Fig.4. They used a finite-element-type model with a grid node at the contact point that required them to impose a "slip" boundary condition on the wall near that node.

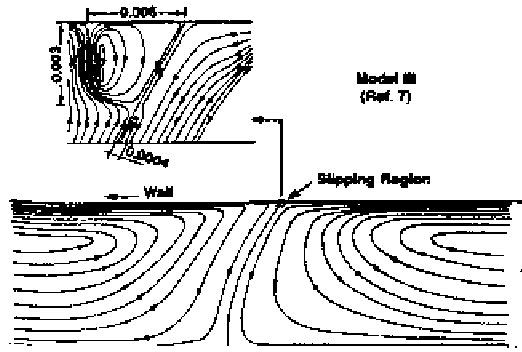

Figure 4. Results from Sheng and Zhou[6] showing recirculation in slip zone.

Sheng and Zhou tried several slip prescriptions that all gave rise to a small recirculation zone adjacent to the contact line (see blowup in Fig.4). They comment: "In the slipping region ... different models exhibit different behaviors" and elsewhere "At the macroscopic level, the different slipping models all exhibit qualitatively the same behavior." These comments indicate that the computed recirculation is a result of the slip model and probably has no physical significance.

The direction of the recirculation velocity at the wall is opposite to the velocity of the wall. This could not happen with a no-slip boundary condition. In any case, slip induced recirculation does not resolve the issue of conflicting boundary conditions at the contact line for there is still a tangential velocity discontinuity outside the recirculation zone.

When we apply the VOF numerical model to this type of flow a different picture of what happens at the contact line emerges. Figure 5 shows a computed flow field at steady conditions that was produced by the commercial FLOW-3D® program[4]. There are no recirculation zones near the contact line. Instead, there is a region of relative stagnation (dark region) that exists about the two-fluid interface. This region is thickest at the center of the tube and tapers to zero at the wall.

A stagnation region about the interface solves the problem of the tangential flow discontinuity observed in the Sheng and Zhou result, because there is no flow along the interface. In the neighborhood of the contact line the flow being pulled down by the moving wall is deflected at the contact line into the interior of the tube. A similar, but reverse, deflection occurs in the liquid below the interface.

Above and below the interface the two fluids have oppositely directed tangential flows. This opposition resolves itself by the generation of a zero velocity boundary layer region.

We could approximate the flow in the upper liquid by replacing the lower fluid with a rigid boundary. For example, a knife-edge pulled along the wall would generate this situation. The knife-edge deflects the flow off the wall, and also causes a boundary layer of zero flow velocity to develop along its surface, see Fig.6.

What the VOF computation shows then, is a simple flow pattern that is consistent with conditions along the interface and makes good sense in the neighborhood of the contact line. It is unnecessary to introduce local slip or other ad hoc mechanisms to obtain this solution. The dynamic contact angle at the wall is about 105°, which differs from the static angle of 100° and results directly from the computation.

There remains a question of what actually happens precisely at the contact line. In the knife-edge analogy there would have to be an infinite pressure right at the contact point to deflect flow off the wall and along the knife blade. In reality, some small amount of fluid probably escapes the blade and remains on the wall. Of course the knife and wall cannot be perfectly smooth and cannot have perfect contact. A locally high pressure could cause elastic deflections in the wall and/or blade. None of these phenomena are considered in our model because we are not seeking answers about the flow on such small scales.

5. REFERENCES

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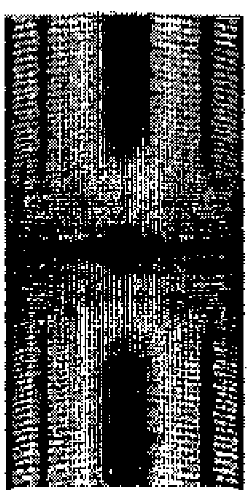

Figure 5. Computed capillary rise using VOF method. No recirculation regions are found near contact line. The flow on either side of the contact line is similar to a corner flow.

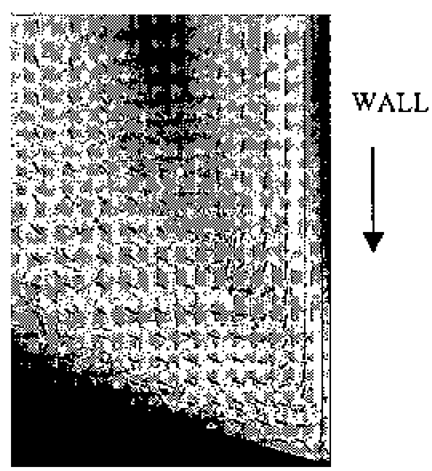

Figure 6. Knife-edge flow analogy in vicinity of contact line corner.