Simulation of Transient and Three-Dimensional Coating Flows Using a Volume-of-Fluid Technique

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Abstract

Slide-coating flow is widely used for the manufacturing of precision film-coating products. Considerable effort is being devoted toward a better understanding of slide-coating processes in hopes of increasing coating speeds and improving the performance of coated film. It has been demonstrated, for example Chen[1] , that increasing coating speeds beyond well defined limits can result in a complete breakdown of the coating bead. In this paper we present simulation results of slide-coating flows obtained from a computational method capable of describing arbitrary, three-dimensional and time-dependent deformations of fluid surfaces. The method, which is available in the commercial program[2], uses a fixed grid through which fluid is tracked by a Volume-of-Fluid (VOF) technique[3,4]. Surface tension, wall adhesion, fluid momentum, and viscous stresses are fully accounted for in our analysis.

The basic method is illustrated through comparisons with dip-coating data[5]. Then we present a discussion on how contact lines and dynamic contact angles are implicitly treated in our method. Because we use a VOF technique, we need only sum the forces acting on each control volume containing fluid. The location of contact lines and dynamic contact angles then arise automatically from the computed balance of forces. Our technique is illustrated with examples of startup and bead-breakup phenomena in coating flows. As will be shown, for rapid processes our approach offers efficiency and robustness for the simulation of coating process design and optimization that is difficult to achieve with conventional analysis methods.

Introduction

All coating processes involve some sort of startup period in which the coating material undergoes large deformations before achieving steady conditions. A good characterization of the startup process is often important for reducing waste and ensuring that the process operates within the desired limits.

A similar understanding of the transient response of coating flows to a variety of perturbations is also desirable so that a breakdown of the coating bead and non-uniformities in coating can be avoided.

Because the dynamics of coating flows is generally non-linear and because it involves the coupled interaction of a variety of competing physical processes, it is necessary to resort to special computational tools to perform theoretical investigations.

The advantage of the modeling tool we have selected for this work is that it uses a robust numerical technique, the Volume-of-Fluid (VOF) method, which has the power to track arbitrary fluid deformations through a fixed grid. The manner in which this is done, along with other features of the program important for coating flow analysis are described in the next section.

Overview of Numerical Method

The numerical program, ***FLOW-3D®***, employed here has its origin in the Marker-and-Cell (MAC) method[6] developed at the Los Alamos National Laboratory in the mid 1960s. Many improvements to the original MAC method have been made over the years. Of most interest for the present application is the replacement of the discrete marker particles by a continuous Volume-of-Fluid function to locate fluid regions. In the VOF method a fixed grid of rectangular control volumes

is constructed that covers the computational region of interest. For each control volume a number, F, is kept to denote the fraction of that volume that is occupied by liquid.

In addition to use of the F function, the VOF method also uses special numerical techniques to advect the F function through the fixed grid of rectangular cells in a way that retains sharp liquid-gas interfaces. And, finally, the VOF method employs a carefully implemented set of free-surface boundary conditions to satisfy the proper normal and tangential stress conditions at interfaces.

Another special feature of our approach is the way in which we define complex geometric regions. Obstacles are embedded in the fixed grid by allowing them to block portions of control volumes. The fractional areas and volumes open for flow in each control volume are stored as the geometry representation. This method, referred to as the FAVOR method[7], automatically incorporates the geometry into the discretized equations for mass, momentum and energy.

Using the VOF and FAVOR methods saves time and effort because there is no complicated grid generation process needed to define the geometry and initial fluid configuration for a coating problem.

In the next section we illustrate the utility of the basic numerical method with an application to dip coating on a flat sheet.

Dip Coating - A Validation Test

Lee and Tallmadge[8,9] have conducted an extensive investigation into the process of dip coating on flat sheets withdrawn vertically from a liquid bath. This process is widely used in a variety of commercial applications. Their study focused on two-dimensional flow (i.e., no edge effects) and consisted of an analytical surface profile containing empirical parameters fit to their experimental data. Experimental data was collected for capillary numbers between 0.085 and 23.9, with Reynolds numbers ranging from 0.044 to 12.7. Experimental data for film thickness had an error estimated to be less than or about 10%.

The computational model for this experiment is extremely simple as it consists of a rectangular bath with the left side wall given a vertical (tangential) velocity equal to that of the sheet to be coated. Initially the coating liquid has a horizontal surface and the sheet is given an impulsive start, see Fig. 1c.

A number of different capillary number cases were simulated and in all cases the predicted film thicknesses were well within the experimental error. As an example, consider the case corresponding to capillary number 1.17. The sheet was withdrawn from the bath (viscous lubricating oil having a density of 0.885 gm/cc, surface tension 32.7 dynes/cm and viscosity 1159.4 cp) at 3.31 cm/s.

We used a bath width of 2.5 cm and depth of 2.0 cm (35 by 25 grid cells). A 2.0 cm region above the bath was included in the model to capture the film flow (requiring an additional 25 cells vertically). The right side of the bath was an open boundary where the fluid height was maintained constant, the pressure was hydrostatic and flow was allowed to enter the computational region, but did so by having to start from rest. This, so called, "stagnation" boundary condition is a good approximation to a horizontally infinite bath provided it is sufficiently far to the right of the moving sheet. Several computations were done to establish the width of the bath that needed to be modeled, and it was found that film thickness is not very sensitive to this width, a result also found in the experiments.

Figure 1a shows the initial condition, Fig. 1b one snapshot of the computed transient and Fig. 1c the final steady-state result. The shape of the tip of the liquid being initially drawn up by the sheet depends on the static contact angle (i.e., adhesion between sheet and liquid) and was arbitrarily taken to be 10 degrees. As the liquid is drawn up, a depression wave moves to the right as a signal to the remainder of the bath that a flow must be started toward the sheet to replace the liquid film being withdrawn. Steady conditions are reached in about 5.0 seconds. The film thickness was computed to be 0.145 cm, which is in excellent agreement with the measured value of 0.142 cm.

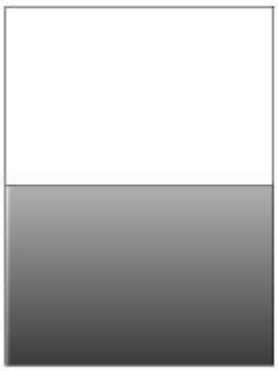

Figure 1a: Dip coating (initial condition)

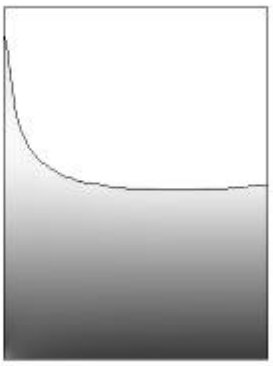

Figure 1b: Dip coating (t = 0.4 seconds)

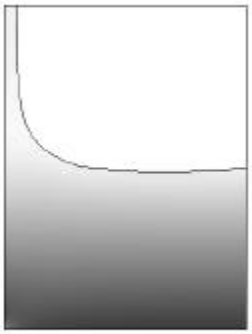

Figure 1c: Dip coating (t=5.0 seconds)

Contact Lines and Dynamic Contact Angles

Dip coating is relatively simple in that, once established, it involves no contact line defining a fluid/solid wetting boundary. In other situations such as slide coating, contact lines exist where fluid leaves the slide and where it makes

contact with the surface of the substrate to be coated. A considerable literature exists[8,9,10] describing experimental and theoretical studies of possible dynamical processes occurring at contact lines.

The Problem

Simply put, it's not obvious how a stationary contact line can exist and at the same time be attached to the moving surface. In a computational model this paradox is exposed in the process of assigning boundary conditions to the coating fluid. For example, in the finite-element method it is natural to place a node line coincident with the contact line, since this defines a limit of the fluid surface. However, this line is also coincident with the solid and free (air) surfaces.

On a solid surface a no-slip, viscous type of boundary condition is natural. But under steady flow conditions the contact line is stationary with respect to the moving solid surface. To overcome this contradiction researchers have resorted to a variety of solutions. At the sub-microscopic to mircoscopic scale solutions range from changing the governing equations (e.g., including long-range atomic forces near the contact line) to using modified boundary conditions (e.g., assuming a liquid film already exists on the boundary).

From a macroscopic point of view the no-slip condition is often replaced with an assumption of partial slip plus a specification of the dynamic contact angle.

None of these solutions are completely satisfactory, however, because one would like the dynamic contact angle to be predicted as part of the solution.

Microscopic details of flow processes in the immediate vicinity of a contact line are surely important for an understanding of the fundamental processes of wetting and drying. On the other hand, one hopes they may be unnecessary for engineering applications where the interest is primarily in the macroscopic flow structures associated with coating devices under different operating conditions. For practical, engineering applications it would be most useful if a limited set of parameters were sufficient to characterize fluid/solid interactions.

Contact Lines and the VOF Method

The use of slip and angle parameters in finite-element models arise because of their requirement for explicit boundary conditions at all boundary nodes. In the VOF control volume method, on the other hand, boundary conditions are not required at contact lines, but rather on control volumes that contain solid and/or fluid surfaces.

Fluid will fill or empty a control volume depending on the average computed flow velocity (i.e., balance of forces) within that volume. Since the numerical method uses approximations for the conservation of mass, momentum and energy in each control volume, it is natural to ask whether this numerical approach might be able to predict the macroscopic behavior of flow in the vicinity of a contact line with a minimum of additional constraints.

A Test Case

To demonstrate our approach , we consider a special case of a plunging-tape test. In particular, we consider the case of a vertically aligned tape moving into a fluid surface such that the dynamic contact angle is approximately 90° (i.e., the fluid surface remains everywhere nearly horizontal). Experimental data[10] indicates that this condition should occur at a capillary number of about, $Ca=\mu U/\sigma=0.044$.

Figure 2 shows the layout of our control volume method used near the contact line. A staggered arrangement of variables is used in which pressures are located at control volume centers and velocity components are located at face centers to which they are normal. In the control volume containing the contact line the pressure is denoted by p_o. This pressure is computed to include the atmospheric pressure plus a hydrostatic component reflecting the gravitational effect of the height of fluid above or below the center of the cell.

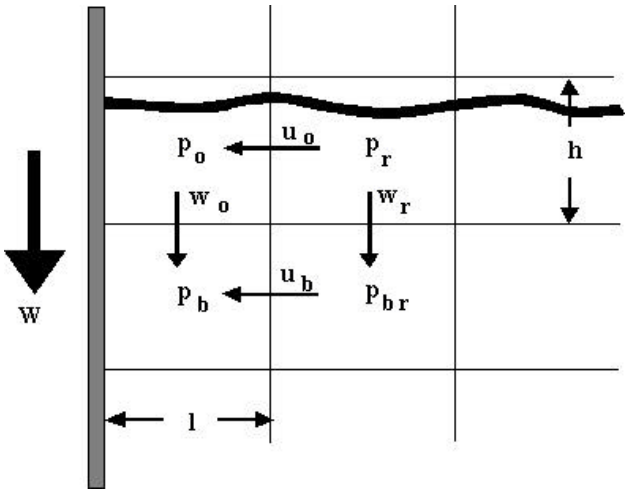

Figure 2:Control volume layout

Surface tension forces acting at the sides of the control volume are also included in the pressure. In the present case of a flat, horizontal surface the tension does not have a vertical component. At the left side of the control volume there is a vertical force contribution from surface tension acting on the solid boundary. This force is computed in terms of the static contact angle, θ_o, through Young's formula,

$$\sigma Cos\theta_o = f_{lg}-f_{ls},$$

where terms on the right side represent the net vertical force per unit length between the fluid and solid (lg on the gas side and ls on the liquid side). This force is included as a boundary stress.

The vertical velocity component w_o at the bottom of the control volume containing the contact line is influenced by the pressure gradient between p_o and p_b, by a gravitational body force and a wall shear stress $2\mu(W-w_o)/l$ with the moving boundary at the left side. Of course, the full momentum equation governing this velocity component also contains contributions from momentum advection and viscous stresses from neighboring velocity components.

At steady flow conditions the amount of liquid in the control volume containing the contact line must not change, which means the volume of liquid flowing out the bottom with velocity w_o must equal the amount flowing in at the right side with velocity u_o.

Even in this geometrically simple case we cannot compute w_o because we don't know the values of the surrounding pressures and velocities. All variables are coupled through mass and momentum conservation relations for the entire set of control volumes covering the region being modeled. If thermal processes are important then an energy conservation equation must be included as well.

Without going into more detail, it should be clear that in this numerical method the contact line location and computed dynamic contact angle, at steady conditions, result from a balance of forces within each control volume. The only parameter used thus far to describe the fluid solid interaction is the static contact angle.

The accuracy of the control volume method, of course, requires the size of the control volumes to be small enough to capture all the important hydrodynamic features, such as surface slope, surface curvature and velocity gradients adjacent to the moving boundary. For example, in the plunging tape example the only characteristic length is that associated with surface tension, $L=\sqrt{\sigma}/ g$, and so we expect the control volume size should be much less than this in order to resolve any macroscopic curvature of the fluid surface.

Computational Results for Test Case

To simplify matters we have used whole numbers for all physical parameters, although they are close to CGS units (e.g., gravity is 1000 instead of 980 cm/s/s). A typical computation might have capillary length L=0.1, capillary number Ca=0.10 and the Reynolds number Re=0.025. The computational region was assumed to extend 4L to the right of the moving wall (plunging tape) and 4L below the fluid surface. At the bottom and right boundaries free-slip wall boundary conditions were used. Gravity was directed vertically downwards.

The computations were checked for convergence and sensitivity in a variety of ways. It should be no surprise that the most noticeable effect on the dynamic contact angle is the resolution of the grid at the contact line. This is the region where there are the most rapid changes occurring in the flow.

For the results shown in Fig. 3 the smallest control volume has an edge length of 0.002, or 50 times smaller than the capillary length L. The flow computed in the vicinity of the contact line is strongly dominated by viscosity. The computed surface in the region extending out from the wall one capillary length is inclined about 1.0° below the horizontal corresponding to an apparent dynamic contact angle of 91.0°. Immediately adjacent to the wall there is an upturn of the surface. This type of localized change in surface slope, right at the contact point, is consistent with many experimental observations [10]. Experimental apparent dynamic contact angles at Ca=0.10 center around 115° ([10], Equ. 4), but with a scatter in the data exceeding 10°. While these initial results could have been a little closer to observations, they nevertheless offer encouragement that dynamic contact angles can be computed with a VOF method.

Additional work is currently underway to further explore to what extent dynamic contact angles can be consistently predicted with the VOF method.

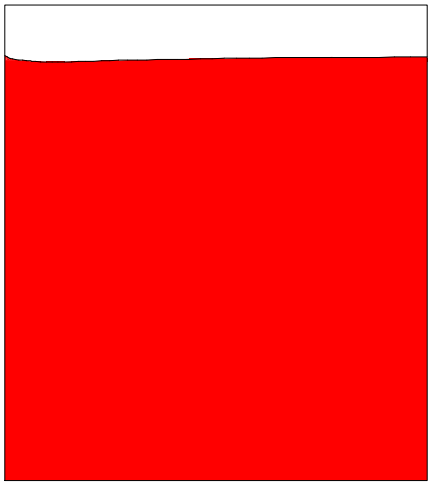

Figure 3a: Plunging tape test (entire domain)

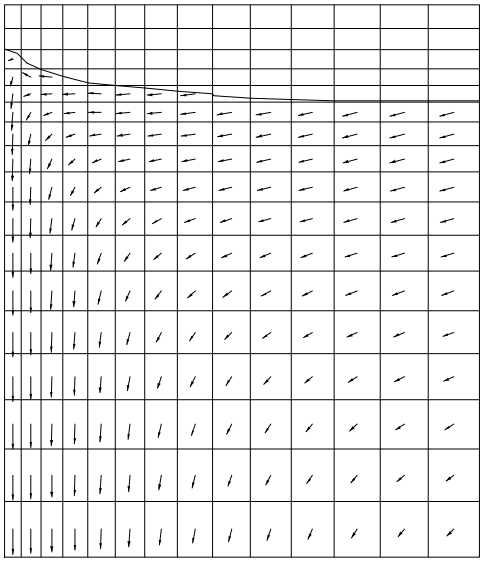

Figure 3b:Plunging tape test (vicinity of free surface, adjacent to wall)

Rivulet Formation in Slide Coating

When manufacturers try to increase coating speeds, they often encounter instabilities in the coating process that destroy the uniformity of the coated product. One such instability is the formation of rivulets, which are stripes of wet and dry regions on the coating substrate. Rivulet formation in slide coating is typically observed to start near an end wall and then propagate across the slide as additional stripes are formed.

To investigate the formation of rivulets we have modeled an end-wall section of a slide coater that is 4000 μm wide. The gap between the tip of the slide and the surface to be coated is 250 μm, and the surface is initially moving upwards at 20.0 cm/s. The end wall of the slide is stationary with respect to the slide. At the other end of the model symmetry

conditions were assumed so that the effective length of the slide is much longer (at least a factor of two) than what is actually computed.

The coating liquid has a density of 1.0 gm/cc, viscosity of μ=12.4 cp, surface tension σ=66.0 dyne/cm, and a static contact angle of 30°. The capillary number for this example was 0.248, which produces a coating thickness of 90 μm under steady conditions.

At the beginning of the simulation there is coating liquid on the slide, but it does not extend to the tip. A constant input of liquid onto the slide surface is made at the upstream boundary of the computation.

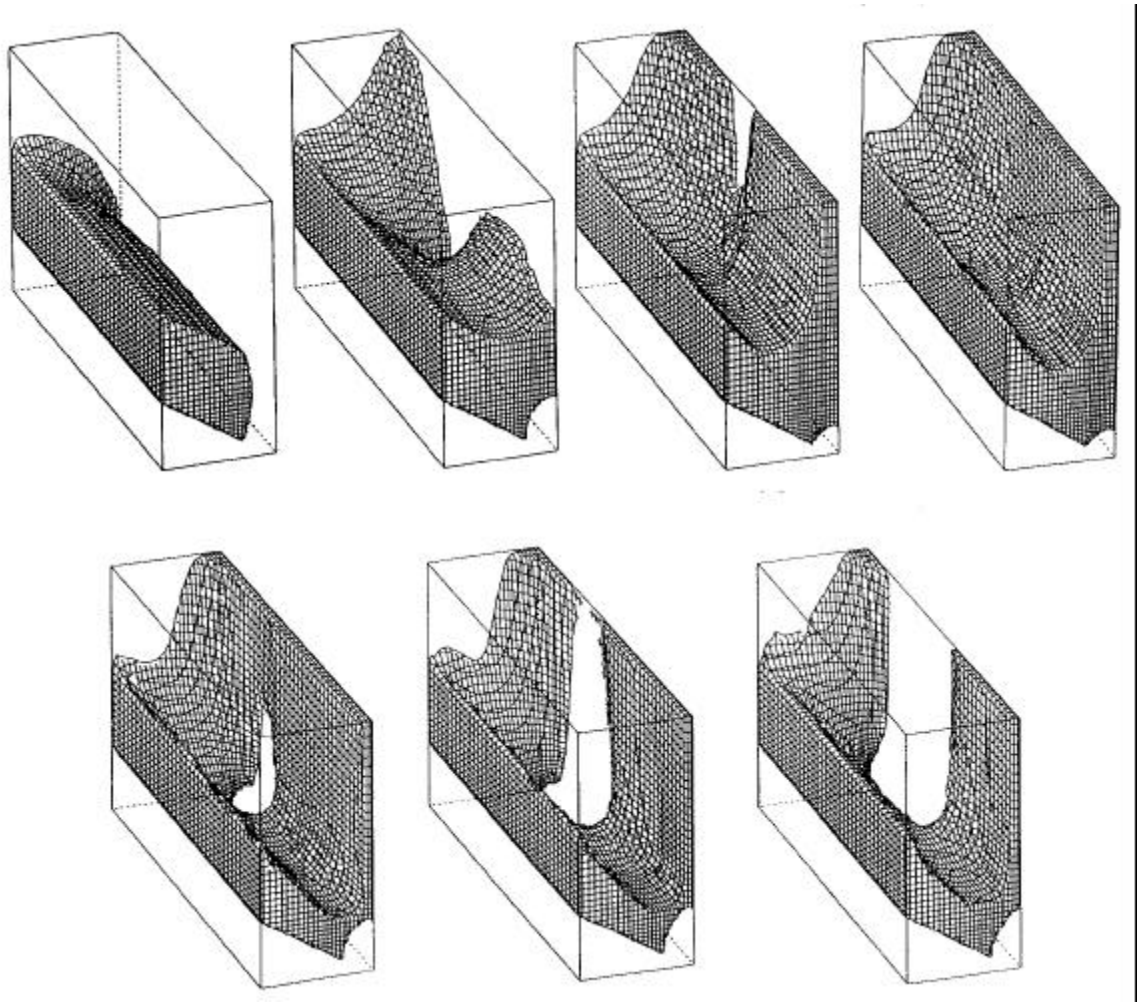

Figure 4: Rivulet Formation (t=0.004, 0.016, 0.026, 0.04, 0.0562, 0.065, and 0.0833 seconds)

Initially, liquid is pulled up the end wall by adhesion before it reaches across the gap and attaches to the coating surface, Fig. 4. This causes a non-uniform deposition of liquid on the moving surface; a capillary wave moves away from the end wall and travels along the lip of the slide. After about 26 ms liquid has reached the coating surface along the entire length of the slide. Uniform coating conditions are reached after approximately 40 ms, although a small capillary is evident close to the symmetry end of the slide, but does not seem to be affecting the coating uniformity.

The speed of the coating surface is impulsively accelerated from 20.0 cm/s to 30.0 cm/s at the 40 ms time point. After a few more milliseconds a tear opens in the coating bead near the stationary end wall. The tear appears to arise because the increased coating speed attempts to pull more liquid away from the tip of the slide, but the slower moving liquid near the end wall cannot respond as quickly to the thinning action. Once the tear appears, surface tension forces contract the liquid surfaces on either side of the tear causing a rivulet with vertical sides to be generated on the coating surface (last frame in Fig. 4).

It is likely that the ultimate rivulet size, which approaches the symmetry end boundary, is being controlled by the limited extent of the simulation, however, the transition in flow conditions from the stationary end wall out into the

remainder of the slide is adequately resolved. The initiation of the tear in this region occurs because of the strong three-dimensional curvature of the surface and end-wall viscous effects.

Summary

We have described a Volume of Fluid technique for the analysis of coating flows. The technique was first verified by simulation of a simple dip-coating experiment. Then a plunging tape test was simulated to show that dynamic contact angles could be reasonably predicted using the control volume method. Finally, the method was applied to rivulet formation in a three-dimensional simulation of slide-coating. The successful completion of these tests suggests that the VOF approach as implemented in our program may be useful for coating process design and optimization applications.

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Presented by John L. Ditter at the 50th Annual Conference of the Society for Imaging Science and Technology, 18-23 May, 1997.

Figure 3 data revised 5/28/97.