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Effective slip in numerical calculations of moving-contact-line problems

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Abstract. For many coating flows, the profile thickness h, near the front of the coating film, is governed by a third-order ordinary differential equation of the form $h''' = f(h)$, for some given $f(h)$. We consider here the case of dry wall coating which allows for slip in the vicinity of the moving contact-line. For this case, one such model equation, due to Greenspan, is $f(h) = -1 + (1 + \alpha)/(h^2 + \alpha)$, where α is the slip coefficient. The equation is solved using a finite difference scheme, with a contact angle boundary condition prescribed at the moving contact-line. Using the maximum thickness of the profile as the control parameter, we show that there is a direct relationship between the effective Greenspan slip coefficient and the grid-spacing of the numerical scheme used to solve the model equation. In doing so, we show that slip is implicitly built into the numerical scheme through the finite grid-spacing. We also show why converged results with finite film thickness cannot be obtained if slip is ignored.

1. Introduction

Many researchers have shown (e.g., Levich 1962; see Tuck and Schwartz 1990 for a recent survey) that a study of coating flow problems, where surface tension forces are significant, very often involves solving third-order ordinary differential equations for the film coating thickness in a region local to the moving front of the coating film. For example, in the case of a thin film draining under gravity down a dry vertical wall, as shown in Fig. 1, the equation governing the profile thickness near the front of the film is given by

$$h''' = -1 + \frac{1}{h^2}\,, \tag{1.1}$$

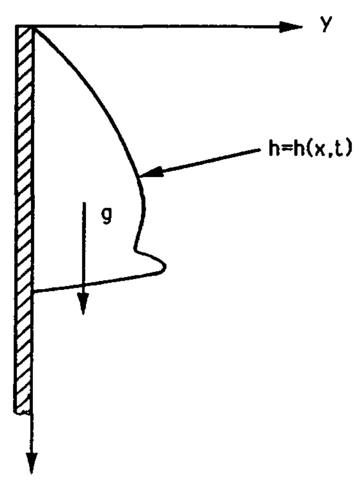

Fig. 1. Drop draining down a vertical wall under gravity.

where $h(x)$ is the non-dimensinal profile thickness, measured in multiples of the profile thickness upstream of the front, h_F. The non-dimensional spatial variable x, measured along the wall in the direction of propagation of the film, is defined in multiples of $(\sigma h_F/\rho g)^{1/3}$ where σ is the surface tension of the fluid, ρ is the fluid density and g is acceleration due to gravity.

In a recent study of wet-wall coating, where the solid substrate is pre-wetted with a thin film of non-dimensional thickness δ, Moriarty et al. (1991) have shown that (1.1), which is the limiting case as $\delta \rightarrow 0$, is also the model equation for two other coating flows, these being spin-coating and spray-coating. The distinction between each coating mechanism on the meniscus length scale at the front of the film enters only through the non-dimensionalisation of the spatial variable x. Thus study of (1.1) is relevant to many coating flows and is not restricted to just one coating process alone.

Despite the seeming simplicity of (1.1), there are some fundamental difficulties in its solution, since it becomes singular at the contact-line, where $h = 0$. The genesis of this singularity is entirely physical, and lies in the so-called 'contact-line paradox'; the classical no-slip boundary condition being in direct conflict with the requirement of contact-line movement.

One way of circumventing the contact-line singularity is to introduce a slip coefficient into the governing equation which relaxes the no-slip condition in a small region local to the contact-line. This idea was used by Greenspan (1978), when he postulated that there was some small amount of slip in the vicinity of the contact-line. The slip he proposed was of Navier-type (see, e.g., Panton 1984), and so was proportional to the local velocity gradient at the contact-line; the factor of proportionality being $\alpha/3h$ where α is a non-dimensional slip coefficient and is generally a small number. Hocking (1981) also added a form of slip in to the equation; his slip formulation weakened the singularity, rather than removed it.

Despite the formidable nature of (1.1) when $h = 0$, it is nevertheless possible to compute free surface profiles by ignoring the singularity altogether. Infinite derivatives at the contact-line, which would normally be a result of the singularity there, are avoided because there is always some amount of numerical slip implicit to any numerical scheme used to solve (1.1). The singularity only becomes apparent through the fact that convergence under spatial refinement cannot be established. This numerical manifestation arises due to the fact that the governing equation is solved at discrete points on the flow domain, i.e. equation (1.1) is satisfied at a point close to the contact-line but not at the contact-line itself.

It has been suggested to us (Davis 1988) that this implicit numerical slip is a function of the numerical grid-spacing, Δx. One way of thinking about it is that the no-slip condition can only be enforced at discrete nodes in the flow domain. Thus, in the space *between* the nodes, the no-slip condition is not enforced. It is in this space, of length Δx, that the contact-line is free to move, so that the smaller the Δx, the smaller the amount of movement – or slip. In the present work, we show that there is a direct relationship between effective slip and numerical grid-spacing.

2. Procedure

Following Greenspan's formulation, the governing equation for coating profiles, with the addition of slip, is given by

$$h''' = -1 + \frac{1+\alpha}{h^2+\alpha}\,, \tag{2.1}$$

which is a more general form of (1.1), reducing to (1.1) when $\alpha = 0$. The finite difference scheme used to approximate the derivative in (2.1) is $O(\Delta x)$ accurate, so that (2.1) reduces to the singular problem of (1.1) if $\alpha < O(\Delta x) \ll 1$. In other words, for all non-zero α, with $\alpha > O(\Delta x)$ so that the numerical scheme can 'see' the slip, the stress singularity at the contact-line is alleviated.

In order to ascertain the relationship between the slip coefficient α and the numerical grid-spacing Δx, we use the maximum thickness of the profile (called the overshoot) as the control parameter. Proceeding in two steps, we firstly solve (2.1) for a given grid-spacing and no slip (i.e. $\alpha = 0$), to determine the overshoot. We then solve (2.1) with some finite amount of slip, and a grid-spacing $\Delta x \ll \alpha$ so that all results are converged, iterating on α to determine the degree of slip required to produce the same amount of overshoot as for the zero slip case.

Ordinarily, (2.1) would be solved as an initial value problem using a Runge–Kutta formulation, with the initial condition being a perturbation from the linearized problem far upstream of the contact-line. However, this method requires input of the small perturbation parameter; the contact angle at the contact-line comes out as part of the solution and thus cannot be specified *a priori*. Solution of a general class of these problems using a Runge–Kutta method is discussed in detail by Tuck and Schwartz (1990).

Since the contact angle is a monotonically increasing function of the overshoot (Tuck and Schwartz 1990), in order to obtain meaningful results, all computations must be done for a constant contact angle ϕ. This requires us to solve (2.1) as a boundary value problem using a finite-difference scheme, so that the contact angle can be prescribed.

Two of the boundary conditions are imposed at the contact line, and are

$$h = 0$$

and

$$h' = -\tan\phi\,.$$

Note here that ϕ is the contact angle for the nondimensional problem. The correspondence between this and the physical contact angle ϕ_p is $\tan\phi = (\sigma/\rho g h_F^2)^{1/3}\tan\phi_p$.

The third boundary condition, derived by Goodwin and Homsy (1990), is an asymptotic boundary condition far upstream of the contact line,

$$h'' - \left(\frac{2}{1+\alpha}\right)^{1/3} h' + \left(\frac{2}{1+\alpha}\right)^{2/3}(h-1) = 0\,.$$

This boundary condition is in agreement with Tuck and Schwartz's initial condition, but does not require the input of a small parameter.

3. The numerical scheme and results

Equation (2.1) is solved by dividing the flow domain into n discrete points, and using low-order central differences. The profile thickness $h(x)$ is evaluated at the midpoint of the nodes, so that (2.1) is not actually solved at the contact-line itself. Thus, in discrete form (2.1) can be written

$$h(i+2)^{k+1} - 3h(i+1)^{k+1} + 3h(i)^{k+1} - h(i-1)^{k+1} - \Delta x^3\left[-1 + \frac{4(1+\alpha)}{(h(i)^k + h(i+1)^k)^2 + 4\alpha}\right] = 0 \tag{3.1}$$

where the k superscript refers to the k^{th} iteration, and i is the nodal reference point, with $i = n$ corresponding to the nodal point at the contact-line. A schemata is illustrated in Fig. 2.

In the above equation, the h^2 term is evaluated at the previous iteration level; thus we have a system of n linear equations in n unknowns to be solved at each iteration. The resultant coefficient matrix is banded with a bandwidth of four, and a pentadiagonal solver is used to calculate $h(i)$ at each iteration. A Newton–Raphson scheme is used to perform the iterations, and convergence is typically established in five iterations. Computations were performed on an IBM 3090, using between 10^3 and 10^4 nodal points.

All calculations were done for a contact angle of 45 degrees, with respect to the nondimensional variables. This would correspond to a physical contact angle such that $\tan \phi_p = (\sigma/\rho g h_F^2)^{-1/3}$.

Figure 3 shows a comparison between the profile calculated without slip, $\alpha = 0$, and grid-spacing $\Delta x = 0.05$, to that profile calculated with a finite degree of slip, $\alpha = 0.0064$, and a grid-spacing $\Delta x = 0.0002$. In the latter (finite-slip) calculation, the amount of slip was chosen to provide the same overshoot as in the zero-slip case, whilst the grid-spacing was chosen small enough to ensure converged results. Note that the zero-slip calculations are non-convergent solutions of the singular problem (2.1) with $\alpha = 0$. The finite-slip calculations, on the other hand, are converged solutions to the well-posed problem (2.1), when $\alpha \neq 0$. The two curves are indistinguishable, with agreement being to within three decimal places.

A graph of slip coefficient versus grid-spacing for a contact angle $\phi = 45°$ is denoted by the curve with symbols in Fig. 4. The solid line pertains to the polynomial,

$$\alpha = 0.0173\,\Delta x + 2.24(\Delta x)^2\,, \tag{3.2}$$

which is a good fit to the numerical data.

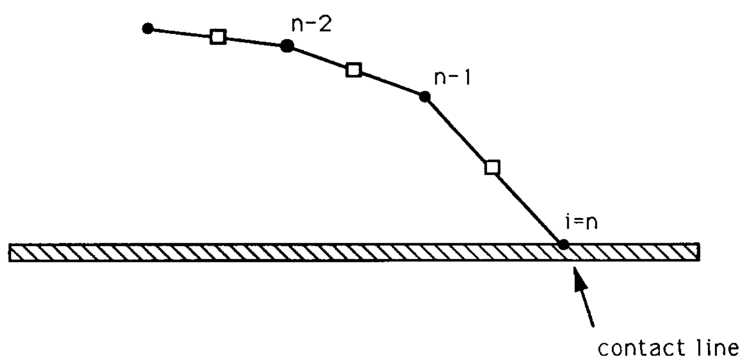

Fig. 2. Schematic of the numerical scheme. Circles represent element end points, and squares represent collocation points, where (3.1) is solved. Note that (3.1) is not solved at the contact-line itself.

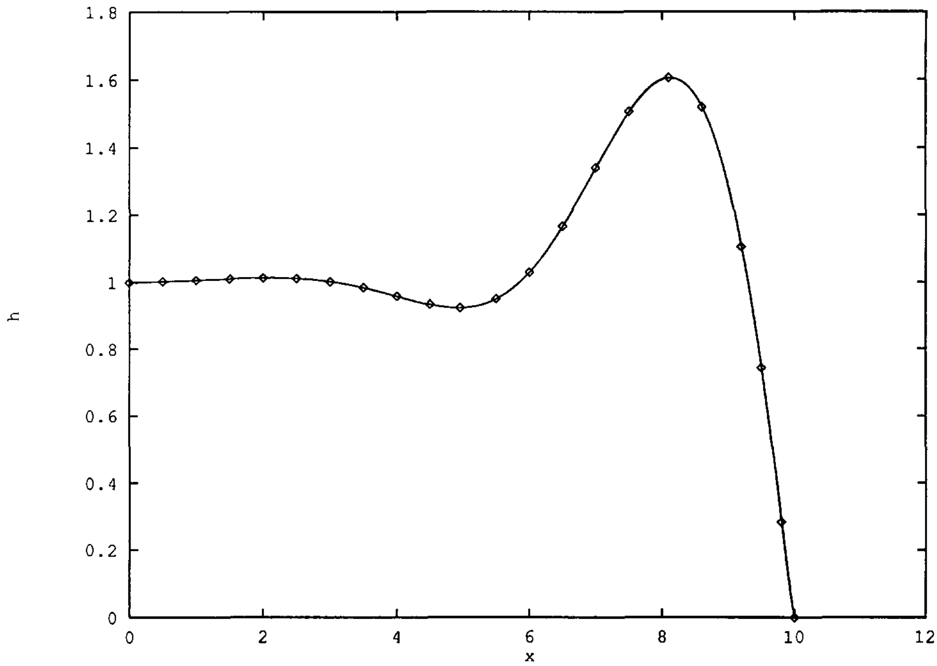

Fig. 3. Comparison of computed profiles with and without slip. The zero-slip model (symbols) is computed with a grid-spacing of $\Delta x = 0.05$. The finite-slip ($\alpha = 0.0064$) model, denoted by the solid line, is converged.

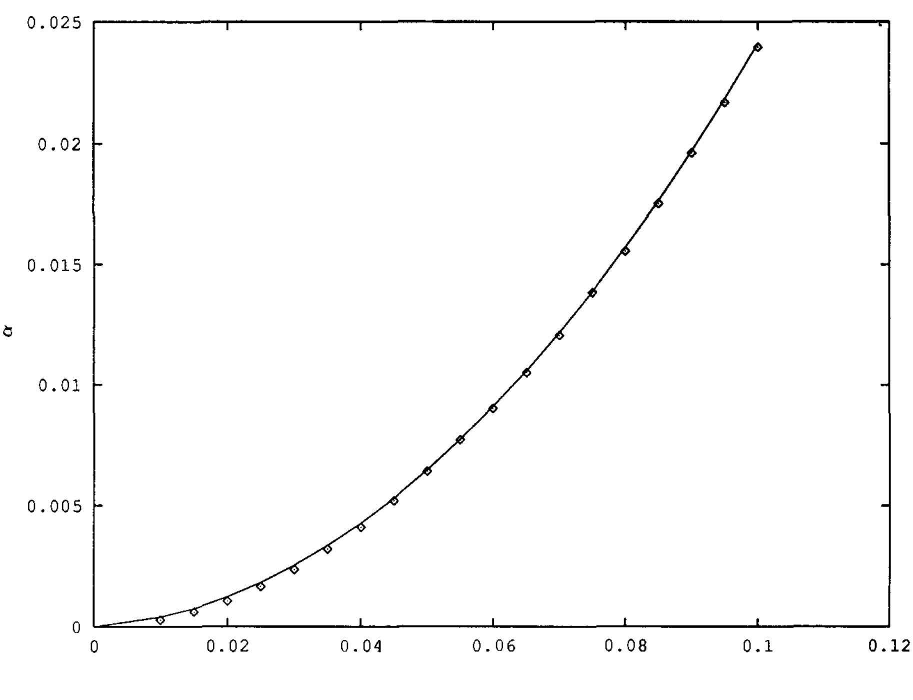

Fig. 4. Slip coefficient α vs grid-spacing Δx (symbols) for a contact angle of $\phi = 45°$. The solid line pertains to the polynomial (3.2).

The fact that the α vs Δx curve passes through the origin is important. It shows definitively that, in order to obtain finite overshoot and converged results with $\alpha = 0$, a grid-spacing $\Delta x = 0$ would be required. In other words, converged finite results, if slip is ignored, can never be obtained. This is the numerical manifestation of the non-integrable force singularity at a moving contact-line when slip is not permitted. If α is set equal to zero, whilst Δx is made small, the overshoot will increase monotonically to infinity.

Since the overshoot is a function of the contact angle, (3.2) would not universally describe a relationship begween Δx and α for all contact angles. For example, a plot of α vs Δx for the 60° case is steeper than (3.2), although it still demonstrates the same general trend.

Calculations to look at the relationship between grid-spacing and Hocking's slip coefficient would follow along similar lines to those described in the present work.

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