

Thin static drops with a free attachment boundary

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A thin fluid drop is at rest on a plane vertical surface, supported against gravity by surface tension. The perimeter of the drop is required to lie on a given closed curve, upon which the contact angle is arbitrary. If the drop is of sufficient volume, it can wet the whole area interior to this curve. However, for any given curve, there is a certain critical volume below which this fully wetted configuration is not physically acceptable, the formal solution having negative thickness. It is suggested here as an alternative that the upper portion of the drop, above a free boundary to be determined, must drain completely. Some time-dependent computations in two dimensions are presented to illustrate this draining property. In three dimensions, the static free boundary has zero contact angle, and must be determined as part of the solution. An example solved here is that where the original boundary is a circle, and the free boundary is a non-trivial curve lying inside it, whose shape is found by numerical methods. This problem also has relevance to the shape of a raindrop on a windowpane where surface contamination prevents contact-line motion, and the drop may again be considered to be confined within a prescribed boundary.

1. Introduction

Fluid dynamic problems in which capillary forces play a role are notoriously difficult (see e.g. Dussan V. 1979; de Gennes 1985; Tuck & Schwartz 1990) if there is a moving contact line between the fluid and a solid boundary, since there are apparent paradoxes at the moving points of contact. On the other hand, fluid static problems of this kind have been studied with success for centuries; see Princen (1969) for a useful review and Finn (1988) for a recent analytical study. If the fluid forms a drop or layer on a plane or nearly plane surface, this is a classical elliptic boundary-value problem, and the solution is well defined and uniquely determined.

For example, the problem of a thin layer of fluid on a vertical plane wall under gravity, the wall being of finite extent and fully wetted within a given closed curve, can be reduced to a Dirichlet problem for Laplace's equation, and the solution determined by various means. The properties of the solution include the fact that, in contrast to the situation for a moving contact line, the angle of contact at the fixed contact curve is not prescribed in advance, but rather is determined by the solution. This is also in contrast to some non-fully wet static problems, such as that for a finite-volume drop on an infinite perfectly clean and smooth plane wall, where the extent of wetting is determined by the solution, but the contact angle must be prescribed.

In fact, a smooth wall is somewhat of an idealization, and any irregularity or imperfection will have the tendency to bound the wetted domain, so reducing the problem back to the one of interest here. For example, a commonly observed phenomenon is a raindrop apparently at rest on a dirty windowpane. Even though

the glass is vertical, the drop can be in equilibrium against gravity because the contact angle, where the edge of the drop meets the glass, can vary around the periphery and is, in general, larger on the lower portion of this boundary. Thus the net surface-tension force on the droplet is upward, balancing the weight. Because the glass is contaminated, the contact angle is not uniquely given; rather it is merely constrained to lie in an interval between the so-called receding and advancing angles. The difference between these angles is a measure of contact angle hysteresis (Schwartz & Garoff 1985), an effect associated with variable surface energy density on a microscopically 'spotted' surface. Similar effects can be shown to occur on clean but microscopically rough surfaces.

When the hysteresis is large, and there are effectively no bounds on contact angle, the problem can thus be simplified to one for a drop on a perfectly plane wall, where the perimeter curve of the drop is given, whereas the contact angle variation needs to be found as part of the solution. For a perimeter of given shape, formal solutions to this static problem will always exist in which the wall is wetted everywhere inside that perimeter.

However, these solutions are not always physically acceptable. In particular, when the drop is very thin, they do not necessarily have everywhere positive thickness. This is not acceptable if the wall is plane and impermeable. What is the alternative?

We suggest here that when the volume of fluid in the drop is less than a certain critical value, a steady-state solution with positive thickness will still be possible, but with the liquid occupying only the lower portion of the original domain. On the upper portion of the domain, the layer thickness is identically zero. In effect, the upper portion has de-wetted.

On the to-be-determined free boundary separating these two regions, we have an additional boundary condition, namely that the normal gradient of the elevation, or equivalently the contact angle, is zero. This condition follows from the realization that the steady free-boundary problem is the ultimate state following a transient motion of the fluid, when the 'dry' portion has drained to vanishing thickness in the limit of large time. Examples of such transient computations are presented here for the two-dimensional case, using a lubrication approximation (cf. Schwartz 1989; Moriarty, Schwartz & Tuck 1990) for the dynamics of thin sheets of viscous fluids. In two dimensions, the free-boundary problem for the limiting static solution reduces to determining a single free parameter, namely the reduced length of the wetted segment, and the transient computations confirm that the sheet approaches after a long time the static solution that has the same volume as the initial profile, but on a reduced length such that the upper contact angle is zero.

In three dimensions with an arbitrary given initial drop perimeter, the static problem cannot be solved in closed form when there is de-wetting on a domain that is not known in advance. We present here a numerical solution of the resulting free-boundary problem, for the case when the original perimeter was circular. The results suggest draining of the remaining fluid to the bottom of the circular domain, as the volume of the drop is decreased toward zero. The present numerical method is capable of generating solutions to the problem only so long as about half of the original circular domain remains wetted. However, the drop that de-wets to this extent is already quite thin, having only about 7% of the volume of a drop that is on the verge of first de-wetting at its topmost point.

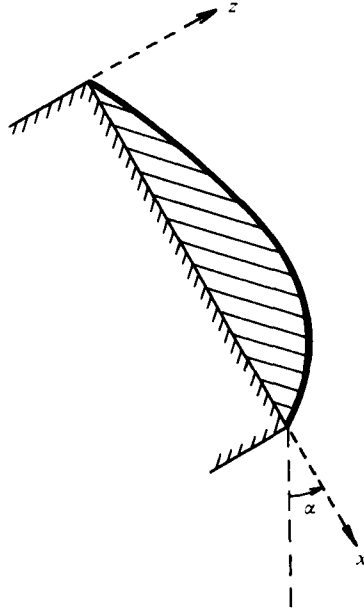


FIGURE 1. Sketch of static drop on a plane wall at a general angle α .

2. Fully wetting solutions

We consider here only thin drops, with thickness $h(x, y)$ satisfying $h_x, h_y \ll 1$. Then if the x -axis makes an angle α to gravity, as indicated in figure 1, static equilibrium of a drop of shape $z = h(x, y)$ is described by

$$-\sigma \nabla^2 h = p_0 + \rho g(x \cos \alpha - h \sin \alpha). \quad (2.1)$$

Equation (2.1) simply expresses balance between the forces of surface tension and gravity, the quantity on the left being mean curvature times surface-tension coefficient σ , and the quantity on the right being hydrostatic pressure, with p_0 an arbitrary constant measuring the hydrostatic pressure at the origin.

For the most part we consider here vertical walls $\alpha = 0$, for which (2.1) is a Poisson equation

$$\nabla^2 h = -\frac{p_0}{\sigma} - \frac{\rho g}{\sigma} x \quad (2.2)$$

with a simple linear function of x as the forcing term, and hence if we write

$$h(x, y) = -\frac{p_0}{2\sigma} x^2 - \frac{\rho g}{6\sigma} x^3 + H(x, y) \quad (2.3)$$

the problem has reduced to one for Laplace's equation in $H(x, y)$.

Consider first the problem of attachment of a drop to a wall of finite extent in the (x, y) -plane, occupying and thus fully wetting the complete interior D of a closed curve C . That is, we have to solve (2.1) in D , subject to the boundary condition

$$h = 0 \quad (x, y) \in C. \quad (2.4)$$

It is assumed that the fluid may make any angle of contact that it chooses with the wall at this boundary C . Then the boundary-value problem (2.1), (2.4) is expected to

have a unique solution for every choice of the arbitrary constant p_0 , which itself can be determined *a posteriori* in terms of the net fluid volume

$$v = \iint_D h(x, y) \, dx \, dy. \quad (2.5)$$

Thus there is a one-parameter family of drops, the single parameter being most suitably taken as the volume v rather than p_0 .

However, there is no guarantee that this unique solution is physically acceptable for all v ; in particular, that $h \geq 0$. Indeed, for sufficiently small v , we must always expect that $h < 0$ at the top of D , i.e. for the most negative values of x .

For example, consider the two-dimensional ($\partial/\partial y \equiv 0$) vertical ($\alpha = 0$) case, where the fluid is assumed to extend from $x = 0$ to $x = l$ and to have unit depth in the y -direction. Then the solution of (2.2) subject to (2.4) is the cubic expression

$$h(x) = x(l-x) \left[\frac{6v}{l^3} - \frac{\rho g}{12\sigma} (l-2x) \right] \quad (2.6)$$

which remains positive near $x = 0$ only if

$$v > \frac{\rho g l^4}{72\sigma} = v_0. \quad (2.7)$$

If (2.7) is violated, there is a region

$$0 < \frac{x}{l} < \frac{1}{2} \left[1 - \frac{72v\sigma}{\rho g l^4} \right] \quad (2.8)$$

where $h < 0$.

Similarly, consider a fluid drop with a circular perimeter, e.g. one attached to the plane vertical end of a circular rod $x^2 + y^2 = a^2$. Then

$$h(x, y) = (a^2 - x^2 - y^2) \left(\frac{2v}{\pi a^4} + \frac{\rho g}{8\sigma} x \right), \quad (2.9)$$

which remains positive near $x = -a$ only if

$$v > \frac{\pi \rho g a^5}{16\sigma} = v_0. \quad (2.10)$$

It is interesting to note that when (2.10) is violated, the boundary between negative and positive h is the horizontal line

$$x = -b; \quad b = \frac{16\sigma v}{\pi \rho g a^4}. \quad (2.11)$$

So, for example, the solution (2.9) is also the exact solution for attachment (with h everywhere positive) of a liquid drop to a closed curve C consisting of such a horizontal line $x = -b$ together with that portion of the circle $x^2 + y^2 = a^2$ lying below it. However, the parameter v in (2.11) is then no longer the actual volume of that drop, since v includes a negative contribution from $x < -b$.

The problem of a non-vertical wall, with $\alpha \neq 0$, can also be solved for some special cases. We quote here only the generalization of (2.10) for a circular rim, namely

$$\frac{v}{v_0} > \frac{64 \cos \alpha}{e^4} \left[1 - \frac{e I_0(\epsilon)}{2 I_1(\epsilon)} \right]^2, \quad (2.12)$$

where v_0 is as given by (2.10), and I_0, I_1 are modified Bessel functions with argument

$$\epsilon = a(\rho g \sin \alpha / \sigma)^{\frac{1}{2}}. \quad (2.13)$$

The quantity on the right of (2.12) tends to 1 as $\alpha, \epsilon \rightarrow 0$, so recovering (2.10) as the wall becomes vertical, and is less than 1 for all $\alpha > 0$, confirming that it is easier to stay fully wet on sloping walls than vertical walls. Since we are interested mainly in the failure of fully wetted solutions, the vertical-wall case is the most sensitive test, and we confine our attention to that case from now on.

3. Transients

The previous discussion shows that static solutions with everywhere-positive thickness h occur above a certain critical volume $v = v_0$. But what happens when $v < v_0$? To answer this question, let us consider unsteady problems, in which an initial drop shape not in steady force balance is allowed to evolve toward an equilibrium shape. In this section, we shall, however, restrict attention to two-dimensional flow, where the thickness of the drop (or sheet) is a function $h = h(x, t)$ of one space dimension x and time t .

For this purpose, we can use a computer program that has been described elsewhere (Schwartz 1989), which was written for the purpose of solving moving contact line problems, but which is equally (in fact better!) suited to solving the present class of problems where the contact line is fixed, and the contact angle is allowed to be determined by the solution.

The (lubrication) equation describing transient motion of a two-dimensional thin sheet of viscous fluid on a vertical plane wall is

$$3\mu h_t = -\frac{\partial}{\partial x}(\rho g h^3 + \sigma h^3 h_{xxx}), \quad (3.1)$$

where μ is the viscosity (see Levich 1962; Tuck & Vanden-Broeck 1984). Notice that when there is no time dependence, this equation integrates once to

$$\rho g + \sigma h_{xxx} = C/h^3 \quad (3.2)$$

for some constant C proportional to the net volume flux in the x -direction. If there is no such flux, then $C = 0$ and (3.2) integrates again to give

$$\rho g x + \sigma h_{xx} = \text{constant}, \quad (3.3)$$

which is the same as (2.2) for the case of no y -dependence.

Hence the time-dependent equation (3.1) certainly possesses a steady-state solution (2.6) that is a solution of (2.2). The question we ask now, is whether that solution is attained in the limit as $t \rightarrow \infty$, when transients have decayed.

It is interesting to note that the derivation of (3.1) as a lubrication approximation to the Navier–Stokes equation is meaningful only if $h \geq 0$. Our numerical method does on occasion allow h to go negative, but this occurs only for relatively coarse spatial discretizations, and as the accuracy of the computations increases, there is little tendency for numerical solutions of (3.1) to exhibit changes in sign of h . Thus with a sufficiently fine grid, starting computations with non-negative $h(x, 0)$ ensures non-negative $h(x, t)$ for all $t > 0$. This experience suggests that such a result could be proved as a formal property of the parabolic partial differential equation (3.1), but let us just accept its reasonableness on physical grounds. In that case, there would seem to be a difficulty if the volume is sub-critical, so that the unique solution (2.6) of (2.2) vanishing at $x = 0$ and $x = l$ takes some negative values of h in $0 < x < l$. It appears that such a solution cannot be attained as a limit of solutions of (3.1).

We have solved (3.1) numerically for a parabolic initial drop shape, i.e. subject to the initial condition

$$h(x, 0) = \frac{6v}{7^3} x(l-x), \quad (3.4)$$

where v is the (conserved) volume. The actual numerical method is similar to that described in Schwartz (1989) and Moriarty *et al.* (1990). In the present case of fixed contact lines, the boundary conditions for this spatially fourth-order partial differential equation are that both h and the volume flux (the quantity inside the parentheses in (3.1)) vanish at each end.

The results show that when $v > v_0$, the solution tends rapidly to the equilibrium result (2.6). When $v < v_0$, the thickness tends to zero in a range $0 < x < x_0$, and tends to the solution (2.6) for $x_0 < x < l$, but scaled so that $x = x_0$ is the new origin, and (most important) so that the contact angle at $x = x_0$ is zero, i.e. $h'(x_0) = 0$ as well as $h(x_0) = 0$. This limiting solution is therefore given explicitly as

$$h(x) = (x-x_0)(l-x) \left[\frac{6v}{(l-x_0)^3} - \frac{\rho g}{12\sigma} (l+x_0-2x) \right], \quad (3.5)$$

where x_0 satisfies
$$v = \frac{\rho g (l-x_0)^4}{72\sigma} \quad (3.6)$$

or
$$\frac{v}{v_0} = \left[1 - \frac{x_0}{l} \right]^4. \quad (3.7)$$

For example, computations with $v/v_0 = 0.048$ are shown in figure 2 at various values of time t . In this case, $x_0/l = 0.532$, and the results show h decreasing for $x < 0.532$, at first quite rapidly, but the final draining is very slow.

The implication of these transient computations is that, since for the given volume v on the given length l , there is no possible equilibrium drop with non-negative h , the evolving drop does the best it possibly can under the circumstances, and shortens its own length l to $l-x_0$, choosing x_0 so that the equilibrium solution is (just barely!) feasible. Because this equilibrium solution is exactly critical (on its new length), it has the property that the attachment is tangential at the new upper edge x_0 .

We believe that, although the above result is based only on two-dimensional computations, its main qualitative conclusion is also valid in three dimensions. That is, whenever $v < v_0$ on some initial wetted domain, the drop will undergo a transient evolution toward a steady equilibrium configuration on a reduced wetted domain, with tangential attachment at the 'new' portion of the wetted perimeter. This result seems intuitively sensible, but awaits formal proof, perhaps by variational means.

In summary, given any closed boundary curve C in a vertical plane, there is a critical volume v_0 proportional to $\rho g/\sigma$ and (in three dimensions) to the fifth power of a measure of the linear size of C . For a given volume v of fluid, there will exist a solution corresponding to a steady drop attached everywhere to this boundary curve C , but with $h \geq 0$ only for $v > v_0$. When $v < v_0$, the drop will assume a shape such that it is attached to C only over its lower portion. The upper boundary of the drop will be a free surface F lying entirely inside C , such that not only $h = 0$, but also

$$\frac{\partial h}{\partial n} = 0 \quad (3.8)$$

on F .

The resulting free-boundary problem is sketched in figure 3. We have made no

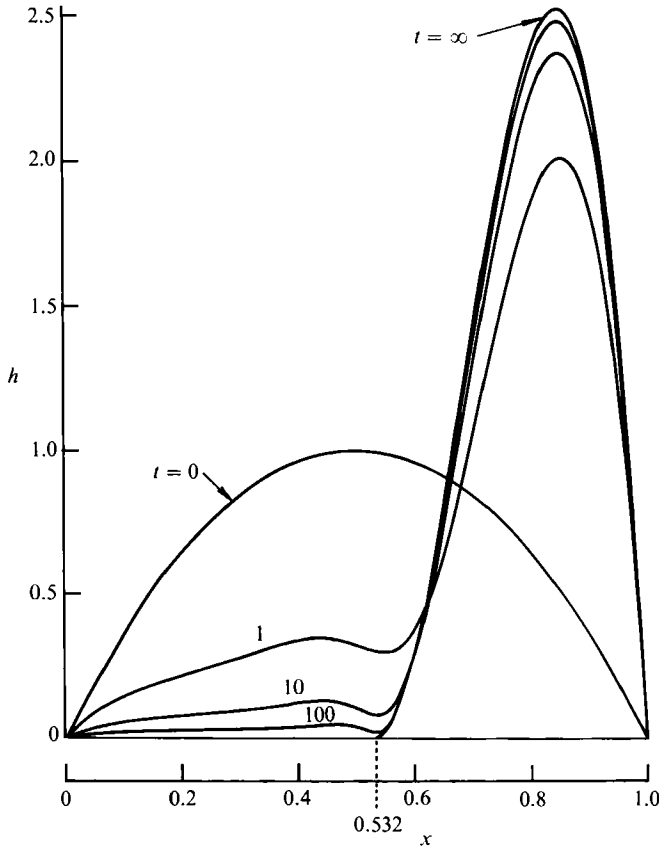


FIGURE 2. Transient computations of draining of an initially parabolic layer with $v/v_0 = 0.048$. The curve labelled $t = \infty$ is the static solution with de-wetting for $x < 0.532$.

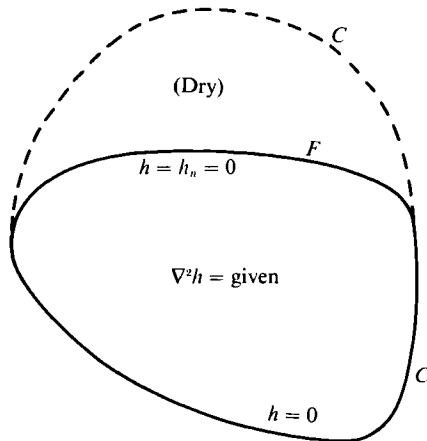


FIGURE 3. Sketch of the free-boundary problem for a general initial perimeter curve C .

attempt to establish any formal analytic properties of this problem, and recommend it to those with such interests. For example, tangency of the attachment of the free boundary F to the original perimeter C , as sketched in figure 3, is purely speculative in the general case. However, we have obtained accurate numerical solutions with this property for the case when C is a circle, which we now describe.

4. Numerical method for a circular boundary

Our aim in the present section is to solve the static problem for $v < v_0$, in the case where the original perimeter curve is a circle on a plane vertical wall, when v_0 is given by (2.10). We use conventional plane polar coordinates (r, θ) , with gravity acting in the x -direction, i.e. in the direction of $\theta = 0$. We assume symmetry about this vertical axis, so that we can confine attention to $0 \leq \theta \leq \pi$. Our task is to solve (2.2) in a region confined by the given circle for $0 \leq \theta \leq \theta_M$, and by a free-boundary curve to be determined inside that circle for $\theta_M \leq \theta \leq \pi$, the angle θ_M at which the free boundary joins the circle being also one of the unknowns.

Let us represent the solution to (2.2) by a polar-coordinate equivalent of (2.3), i.e.

$$h(r, \theta) = -\lambda r^2 \cos^2 \theta - r^3 \cos^3 \theta + \sum_{j=0}^{\infty} a_j r^j \cos j\theta. \quad (4.1)$$

The above applies in a non-dimensional frame of reference such that the circle is $r = 1$, with a thickness scale

$$h_0 = \frac{\rho g a^3}{6\sigma} \quad (4.2)$$

and with the arbitrary constant λ related to p_0 by

$$\lambda = \frac{p_0 a^2}{2h_0 \sigma}. \quad (4.3)$$

The sum in (4.1) is a solution $H(x, y)$ of Laplace's equation, and is the real part of a power series in $x + iy$ about the centre, with unknown coefficients a_j .

In addition, the shape of the free boundary is unknown. Suppose we specify that shape by

$$r = R(\theta) \quad (4.4)$$

for some function $R(\theta)$ to be determined in $\theta_M < \theta \leq \pi$. Hence $R(\theta_M) = 1$, and we may as well set $R(\theta) = 1$ for $0 \leq \theta \leq \theta_M$, too.

Now the attachment boundary condition (2.4) demands

$$0 = -R(\theta)^3 \cos^3 \theta - \lambda R(\theta)^2 \cos^2 \theta + \sum_{j=0}^{\infty} a_j R(\theta)^j \cos j\theta \quad (4.5)$$

for all θ -values, i.e. for $0 \leq \theta \leq \pi$. On the other hand, the zero-contact-angle free-boundary condition (3.8) is satisfied if $\partial h / \partial r = 0$ for only those points on the free boundary, i.e. if

$$0 = -3R(\theta)^2 \cos^3 \theta - 2\lambda R(\theta) \cos^2 \theta + \sum_{j=1}^{\infty} j a_j R(\theta)^{j-1} \cos j\theta \quad (4.6)$$

for $\theta_M \leq \theta \leq \pi$ only. Our task is to choose the unknowns a_j , $R(\theta)$ so that both (4.5) and (4.6) are satisfied.

In fact there is one more unknown, namely the location $\theta = \theta_M$ of the attachment point. However, it is convenient to fix that point as the parameter of the one-parameter family of solutions. In compensation, we must allow λ to be an unknown, and ultimately to allow the solution to determine the volume v of the drop, for each input value of θ_M .

The problem is now easily discretized as follows. Suppose for any integer N , that $\{\theta_j; j = 0, \dots, N\}$ is a set of $N + 1$ increasing values of θ , satisfying $\theta_0 = 0$, $\theta_N = \pi$. Let

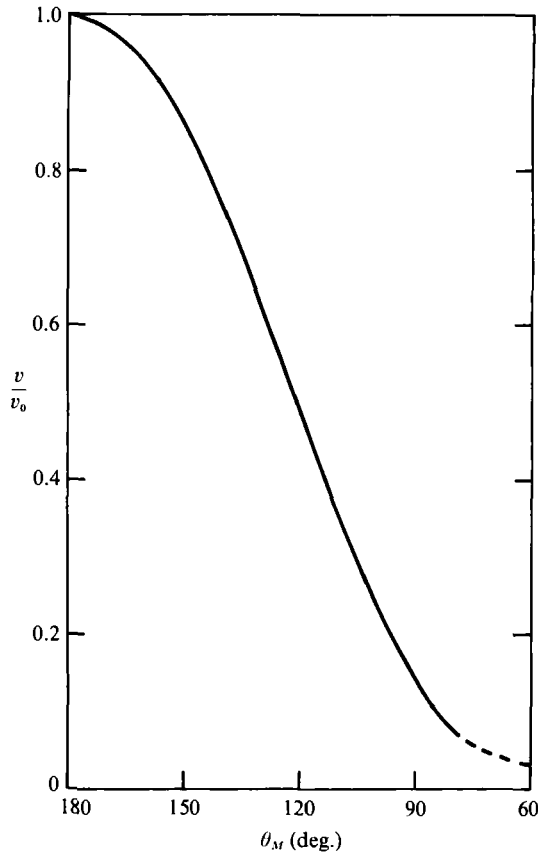


FIGURE 4. Computed relationship between the drop's volume and the polar angle θ_M that locates the point of attachment of the free surface to an initially circular drop perimeter.

the given integer $M < N$ be such that the attachment angle θ_M is a member of that set. Then if the attachment condition (4.5) is enforced for all $N+1$ values of θ_j , and the free-boundary condition (4.6) for the $N-M+1$ values $j = M, M+1, \dots, N$, there result $2N-M+2$ equations.

To balance this number of equations with an equivalent number of unknowns, we truncate the series after the term $j = N$. This will introduce $N+1$ unknown coefficients $a_j, j = 0, \dots, N$. At the same time, we have unknown radii $R(\theta_j)$ at the $N-M$ points $\theta = \theta_{M+1}, \dots, \theta_N$, together with the unknown λ . For convenience, let us redefine for $j > N$

$$a_j = R(\theta_{j-N+M}), \quad j = N+1, \dots, 2N-M \quad (4.7)$$

and
$$a_{2N-M+1} = \lambda. \quad (4.8)$$

Then we have a total of $2N-M+2$ unknowns $a_0, a_1, \dots, a_{2N-M+1}$.

The resulting set of $2N-M+2$ nonlinear equations

$$e_i(a_j) = 0 \quad (4.9)$$

in $2N-M+2$ unknowns (where e_i is the error in the boundary value of h for $i = 0, 1, k, \dots, N$ and of $\partial h / \partial r$ for $i = N+1, N+2, \dots, 2N-M+1$) can then be solved by Newton's method. In fact it is simple enough for all elements of the Jacobian matrix

$$\Omega_{ij} = \frac{\partial e_i}{\partial a_j} \quad (4.10)$$

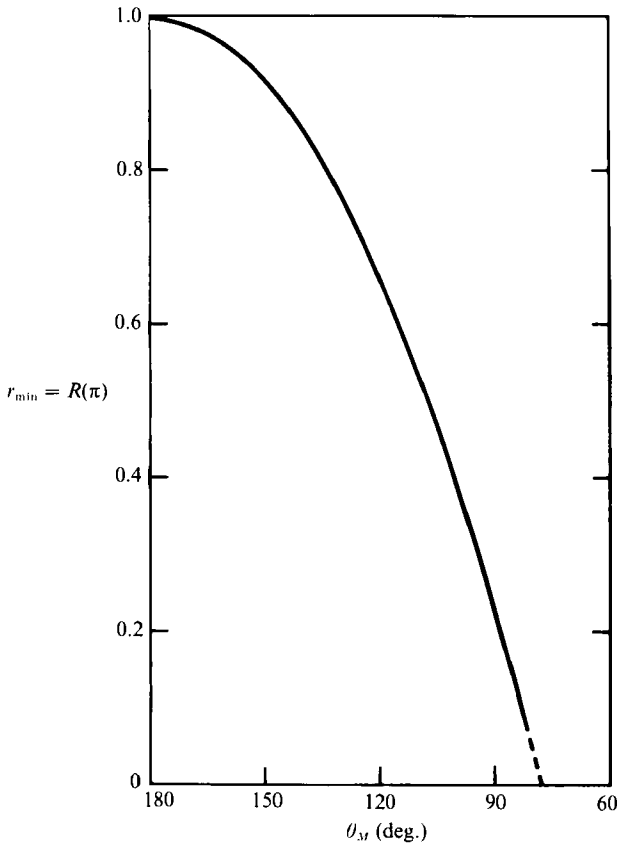


FIGURE 5. Maximum distance $R(\pi)$ of the free surface above the centre of the original circular perimeter, as a function of the attachment angle θ_M .

to be evaluated explicitly, which allows the iteration

$$a \leftarrow a - \Omega^{-1}e \quad (4.11)$$

to proceed rapidly.

5. Results

When $\theta_M \approx \pi$, i.e. the free surface is of small extent and is close to the top of the circle, there is very rapid convergence, and in the limit as $\theta_M \rightarrow \pi$, we find

$$a_0 = a_1 = a_2 = 0.75, \quad a_3 = 0.25, \quad \lambda = 1.5, \quad (5.1)$$

with $a_j = 0$ for $j > 3$, which agrees with the solution (2.9) at the critical volume $v = v_0$ when the drop is just attached to the whole circle.

As we decrease θ_M from π , the Newton iteration converges less rapidly, but adequately until $\theta_M \approx 90^\circ$. Figure 4 shows the volume of the drop as a function of θ_M . Although there is no indication that the family of droplets ceases to exist at any θ_M , the present program is not capable of computing it for θ_M values much below 90° .

In fact, the results suggest on extrapolation (figure 5) that $R(\pi) = 0$ at about $\theta_M = 78^\circ$. That is, the top of the free surface passes through the centre of the original circular boundary at that value of θ_M . The present program, being dependent upon

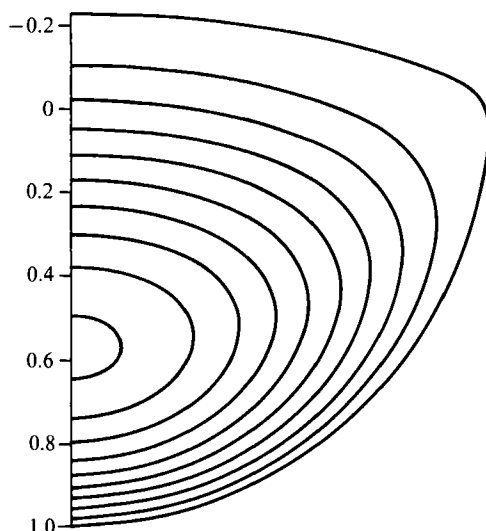


FIGURE 6. Contours of drop thickness for the case $\theta_M = \frac{1}{2}\pi$.

a conventional polar-coordinate representation $r = R(\theta)$ with origin at that centre, must fail whenever $R(\theta) < 0$, but this is an artificial limitation. For example, a relatively simple extension to the present program would be to allow $R(\theta)$ to take prescribed values other than $R(\theta) = 1$ on the known boundary, so solving for attachment to rims of general shape. Then we could solve for circular rims with $\theta_M < 78^\circ$, simply by shifting the origin downward.

Note, however, that the drop's volume is decreasing rapidly as θ_M decreases, and is only about 7% of v_0 at $\theta_M = 78^\circ$. There seems little doubt that as $\theta_M \rightarrow 0$, the trend evident in figure 5 will continue, with $v \rightarrow 0$ smoothly, as the small volume of fluid that is left falls to the very bottom of the circle.

Figure 6 shows contours of $h(x, y)$ at $\theta_M = 90^\circ$. Raindrops on a windowpane look quite like this.

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