J. Fluid Mech. (1996), *vol.* 322, *pp.* 109–129

Flow in an open channel capillary

By L. A. ROMERO AND F. G. YOST
Sandia National Laboratories, Albuquerque, NM 87185-5800, USA

(Received 30 January 1995 and in revised form 19 March 1996)

The problem of capillary-driven flow in a V-shaped surface groove is addressed. A nonlinear diffusion equation for the liquid shape is derived from mass conservation and Poiseuille flow conditions. A similarity transformation for this nonlinear equation is obtained and the resulting ordinary differential equation is solved numerically for appropriate boundary conditions. It is shown that the position of the wetting front is proportional to $(Dt)^{1/2}$ where D is a diffusion coefficient proportional to the ratio of the liquid–vapour surface tension to viscosity and the groove depth, and a function of the contact angle and the groove angle. For flow into the groove from a sessile drop source it is shown that the groove angle must be greater than the contact angle. Certain arbitrarily shaped grooves are also addressed.

1. Introduction

The kinetics of liquid flow into a capillary has been of considerable interest for many years (see e.g. Washburn 1921 and Bell & Cameron 1906) and has received recent attention because of its similarity to flow in porous media and on rough surfaces. Porous media may be considered an ensemble of contorted capillary tubes while rough surfaces may be viewed as contiguous open channel capillaries. Extensive and rapid flow of liquids into surface grooves and scratches on solid substrates has often been observed. Parker & Smoluchowski (1944) immersed grooved iron plates into molten silver and measured the capillary rise into the V-shaped grooves. The grooves were 0.127 mm deep and had basal angles of 60°, 90°, and 120°. The liquid silver rose quickly into the 60° grooves, slowly into the 90° grooves and not at all into the 120° grooves. They also observed preferential spreading in grain boundary grooves that intersected the surface. On iron surfaces that were etched in 50% nitric acid, spreading of liquid silver was so extensive that it eventually covered the entire surface of the iron. Shuttleworth & Bailey (1948) recognized that spreading on a rough surface could be likened to liquid rise in a capillary tube. Under wetting conditions, a tongue of liquid would extend into a surface groove a certain distance that would increase as the groove became deeper and narrower. Spreading across grooves required surmounting an energy barrier. Shepard & Bartell (1953) observed extensive spreading of methanol on grooved paraffin surfaces. Bascom, Cottington & Singleterry (1964) and Cottington, Murphy & Singleterry (1964) saw rapid spreading of various organic fluids on polished stainless steel surfaces. Rapid flow into surface scratches (due to polishing) and the resulting dendritic pattern of fluid was described as 'catastrophic spreading'. Adams (1966) also saw remarkably high spreading rates (several hundred centimetres per second) for silver–copper alloys on copper but did not discuss surface roughness.

Since spreading of liquids is often preceded by flow in surface grooves it is necessary to describe the rate of this flow and the shape of the liquid in the groove. To this end, flow in V-shaped grooves has been modelled by utilizing a method similar to that recently employed by Lenormand & Zarcone (1984). It will be shown that flow distance scales as time to the $\frac{1}{2}$ power, as in most capillary flow problems, and that the magnitude of the flow rate is determined by groove geometry and the ratio of liquid surface tension to viscosity.

2. The equations for a V-shaped groove

Consider a V-shaped groove of depth h_0 in an otherwise smooth, flat surface. A cross-section of such a groove sketched in figure 1 (*a*). When a drop of liquid is placed on this groove, under certain conditions the liquid flows into the groove due to capillary action. It will be assumed that the radius of the liquid drop is much larger than the height of the groove. As the fluid flows into the groove there are two possible situations along the groove. The first possibility is that the fluid only partially wets the sidewalls of the groove cross-section. In this case the height $h(z, t)$ up to which the fluid fills the groove is an independent quantity subject to the restriction $h(z, t) < h_0$. Here z is the axial distance along the groove. In this case the contact angle θ_0 that the liquid makes with the walls of the groove is assumed to be known from the properties of the materials involved or directly from measurement. If the axial variation of the height of the liquid in the groove varies on a length scale much larger than h_0, and the flow is slow enough that forces due to surface tension dominate the inertial and viscous forces, then a cross-section of the free surface of the liquid must be circular.

The second possibility is that the liquid completely wets the sidewalls of most of the groove cross-section. In this case the height $h(z, t)$ must be equal to h_0, but the angle $\theta(z, t)$ that the liquid makes with the walls of the groove is independent of material surface energies provided $\theta(z, t) > \theta_0$. In this case it will be said that the liquid is pinned to the walls of the groove. Once again the cross-section of the free surface of the liquid is assumed to be circular. This situation is sketched in figure 1 (*b*).

The division of the surface into a pinned and an unpinned region is necessitated by our assumption that there is a sharp angle at the top of the groove. If there was a smooth transition at the top of the groove, the angle θ would always be specified, and there would be no pinned region. We elaborate on this point further in §6. In either case the pressure at each point in the groove is assumed to be constant and given by

$$p(z) = \gamma K(z) + p_0, \tag{1}$$

where γ is liquid–vapour surface tension, $K(z)$ is the mean curvature of liquid in the groove, and p_0 is the constant pressure above the liquid in the groove. This expression for the pressure is valid provided the forces due to surface tension are much greater than those due to viscosity (viscous forces are assumed to dominate inertial forces). This will be true provided the capillary number

$$Ca = \frac{U\mu}{\gamma} \ll 1,$$

where U is a characteristic velocity of the fluid flowing through the groove and μ is the dynamic viscosity. If the principal curvature parallel to the groove is neglected the mean curvature becomes

$$K(z) = -\frac{1}{R(z)} = -\frac{\sin(\alpha - \theta)\tan(\alpha)}{h(z, t)}. \tag{2}$$

where θ is viewed as a function of flow distance and time; in equilibrium it is given by $\theta = \theta_0$. The above formula for the radius of curvature is an exercise in trigonometry that can be carried out with the help of figure 1.

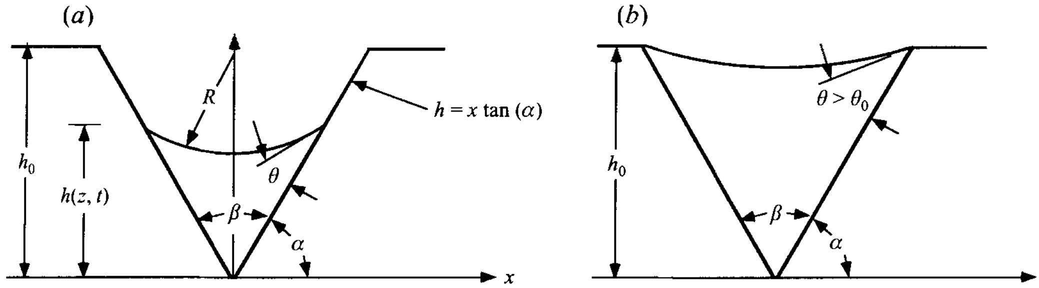

FIGURE 1. (a) A V-shaped groove containing liquid assumed to have a contact angle equal to θ along the entire groove length. (b) A filled groove having a circular surface shape and defining the pinned state.

Our analysis assumes we can ignore the axial contribution to the mean curvature. We should make it clear when this is and is not justifiable. First of all, from (2) we see that this will not be valid if $\alpha = \theta_0$. In this case the only contribution to the mean curvature comes from the neglected axial term. As we shall see, our analysis assumes that $\alpha > \theta_0$, so our assumptions will break down as $\alpha \to \theta_0$.

In general it is assumed that we can neglect the axial contribution to the curvature since the groove is assumed to be very long and thin. The spatial gradients in the axial direction are small compared to the radius of curvature given by (2). However, there are still some regions where this assumption breaks down. At very early times, the drop has not spread far down the groove, so the axial gradients are in fact large compared to the assumed radius of curvature. Also at the boundary between the pinned and unpinned regions, the derivative of the free surface is not continuous. It follows that in this region the assumption also breaks down. Furthermore, in the region very near the drop this assumption will also fail. It is assumed that since these regions of invalidity are confined to very small regions in space and time, that it is reasonable to ignore them.

The volumetric flow rate $q(z,t)$ is given by

$$q(z,t) = \int_{z=const.} U(x,y,z,t)\cdot \boldsymbol{n}\,\mathrm{d}s \qquad (3)$$

where $\boldsymbol{n}$ is the unit normal to the cross-section of the groove. Following the method of Lenormand & Zarcone (1984)), the volumetric flow rate is related to the cross-sectional area, $A(z,t)$, of liquid by the relation

$$\frac{\partial q(z,t)}{\partial z} = -\frac{\partial A(z,t)}{\partial t}. \qquad (4)$$

The cross-sectional area is

$$A(z,t) = h^2(z,t)\hat{A}(\theta(z,t),\alpha), \qquad (5a)$$

where

$$\hat{A}(\theta,\alpha) = \frac{\sin^2(\alpha-\theta)\tan(\alpha) - (\alpha-\theta) + \sin(\alpha-\theta)\cos(\alpha-\theta)}{\tan^2(\alpha)\sin^2(\alpha-\theta)}. \qquad (5b)$$

Note that the function $\hat{A}$ appears to be singular when $\theta = \alpha$, but it is not. In §5 it is shown that the volumetric flow rate can be written as

$$q = -\frac{h^4(z,t)}{\mu}\Gamma(\theta,\alpha)\frac{\partial p}{\partial z}, \qquad (6)$$

where $\Gamma(\theta, \alpha)$ is a positive function. Equation (6) is similar to the classic equation for flow through a circular pipe. In §5 it will be shown that $\Gamma(\theta, \alpha)$ can be calculated by solving Poisson's equation on a cross-sectional slice of the fluid in the groove. The details of the numerical approximation of $\Gamma(\theta, \alpha)$ are given in §5 and Appendix A. For now a very good analytical correlation to the function $\Gamma(\theta, \alpha)$ will be presented. For the special case where $\theta = \alpha$ the value of $\Gamma(\alpha, \alpha)$ can be approximated by the correlation

$$\Gamma(\alpha, \alpha) \approx \frac{1}{6} \frac{\cot^3(a) + 3.4\cot^4(\alpha) + \cot^5(\alpha)}{1 + 3.4\cot(\alpha) + 4\cot^2(\alpha) + 3.4\cot^3(\alpha) + \cot^4(\alpha)}. \tag{7a}$$

When α is varied from 0 to $\pi/2$, (7*a*) predicts $\Gamma(\alpha, \alpha)$ to within 0.1 %. In order to predict $\Gamma(\theta, \alpha)$ the height of the fluid at the midline of the groove is first introduced. This is given by

$$h_c(\theta, \alpha) = h_0\left(1 + \cot(\alpha)\frac{\cos(\alpha - \theta) - 1}{\sin(\alpha - \theta)}\right). \tag{7b}$$

Assuming that $\theta < \alpha$, the correlation

$$\Gamma(\theta, \alpha) \approx \Gamma(\alpha, \alpha)\left(\frac{h_c(\theta, \alpha)}{h_0}\right)^3\left(\frac{\hat{A}(\theta, \alpha)}{\cot(\alpha)}\right)^{1/2} \tag{7c}$$

is employed. This approximate expression for $\Gamma(\theta, \alpha)$ was found to be within 2.5% agreement with the exact numerical calculations provided $\theta < \alpha$.

In order for (6) to be valid it is necessary that the pressure gradient along the axis of the groove changes on a length scale that is large compared to $h(z, t)$. Note that from (1) and (2) the pressure gradient is on the order of $\gamma/[h(z, t) L]$ where L is the characteristic length in the axial direction. From (6) it follows that the average velocity in the groove is on the order of $\gamma h_0/(\mu L)$, and hence $Ca \approx h_0/L$. This shows that the viscous stress does not have much influence on the shape of the free surface provided that the height of the groove is much smaller than its length.

In those parts of the groove where the liquid only partially fills the grove (1), (2), (4), (5) and (6) combine to yield

$$\frac{\partial h^2(z, t)}{\partial t} = \frac{D}{h_0}\frac{\partial}{\partial z}\left\{h^2(z, t)\frac{\partial h(z, t)}{\partial z}\right\}, \tag{8a}$$

where

$$D = \frac{\gamma h_0}{\mu} K(\theta_0, \alpha) \tag{8b}$$

and

$$K(\theta_0, \alpha) = \frac{\Gamma(\theta_0, \alpha)\sin(\alpha - \theta_0)\tan(\alpha)}{\hat{A}(\theta_0, \alpha)}. \tag{8c}$$

Note that this is a nonlinear diffusion equation for $h^2(z, t)$. This is an ill-posed problem if the diffusion coefficient is negative but well posed if $D > 0$ which requires that $\alpha - \theta > 0$. Because α is the angle of a physical surface it can never be greater than $\frac{1}{2}\pi$. Although certain combinations of liquids and solid surfaces can exhibit $\theta > \frac{1}{2}\pi$ (non-wetting conditions) liquids in these systems will not flow into surface grooves. If $\theta < \frac{1}{2}\pi$ flow will commence if α is large enough. Note that when $\alpha - \theta_0$ is positive the free surface of the fluid is concave, and when it is negative the free surface is convex.

In parts of the groove where the cross-section of the groove is completely filled (1), (2), (4), (5) and (6) combined to yield

$$\frac{\partial \hat{A}(\theta(z, t))}{\partial t} = D^* \frac{\partial}{\partial z}\left\{\Gamma(\theta(z, t), \alpha)\cos(\alpha - \theta(z, t))\frac{\partial \theta(z, t)}{\partial z}\right\}, \tag{9a}$$

where

$$D^* = \frac{\gamma h_0}{\mu}\tan(\alpha). \tag{9b}$$

Note that $\partial\hat{A}/\partial\theta > 0$, and $\Gamma(\theta,\alpha)\cos(\alpha-\theta) > 0$ for any physically realizable values of θ and α.

3. The simplified similarity solution

When liquid flows down the groove it is expected that there will be a region in the vicinity of the drop where the fluid is pinned to the walls of the groove. In this section it is assumed that the length of this region is small compared to the wetted length of the groove. This version is considerably simpler and provides a universal solution that applies for all values of the parameters θ_0 and α. In the next section this assumption will be relaxed. The more realistic solution shows that at each instant in time about half of the wetted length of the groove has fluid pinned to the sidewalls.

Let $z = 0$ be the point at which the groove intersects the drop. Considering flow in one direction only (8*a*) is solved with the boundary condition

$$h(0,t) = h_0. \tag{10a}$$

This is a reasonable condition provided the groove is never completely filled with liquid except in a small region around the drop. It is assumed that liquid begins to emerge from the drop perimeter at $t = 0$ which gives the initial condition

$$h(z,0) = 0. \tag{10b}$$

It is also assumed that far down the groove the height of the fluid in a groove approaches zero, that is $h(z,t)\to 0$ as $z\to\infty$. Rather than using this boundary condition the more stringent condition will be used that at any finite time, the total volume of liquid in the groove is finite:

$$\int_0^\infty h^2(z,t)\,\mathrm{d}z < \infty \quad \text{for} \quad t < \infty. \tag{10c}$$

Equation (8*a*), and the conditions (10*a–c*) are all invariant under the change of variables $t\to\lambda^2 t$ and $z\to\lambda z$. This implies that it should be possible to solve this system of equations using the similarity transformation

$$h(z,t) = h_0\,\phi(\eta), \tag{11a}$$

where

$$\eta = \frac{z}{(Dt)^{1/2}}. \tag{11b}$$

Substitution (11*b*) shows that ϕ must satisfy

$$-\tfrac{1}{2}\eta\frac{\mathrm{d}}{\mathrm{d}\eta}(\phi^2) = \frac{\mathrm{d}}{\mathrm{d}\eta}\left(\phi^2\frac{\mathrm{d}\phi}{\mathrm{d}\eta}\right) \tag{12a}$$

$$\phi(0) = 1, \tag{12b}$$

$$\int_0^\infty \phi^2(\eta)\,\mathrm{d}\eta < \infty. \tag{12c}$$

In Appendix B it is shown that it is not possible to solve this system of equations if the function $\phi(\eta)$ approaches zero gradually as $\eta \to \infty$. Instead, the solution must go to zero at a finite value $\eta = \eta_0$, and stay zero. In terms of the original variables $h(z,t)$ and z, this means $h(z,t) = 0$ for $z > z_0(t) = \eta_0(Dt)^{1/2}$. Therefore, the volume flux is zero for $z > z_0(t)$, and hence it must be zero as $z \to z_0(t)$ from below. If this were not the case there would be buildup of a finite amount of fluid in an infinitesimally small region of space. In terms of the similarity variables, the requirement that the flux approach zero at the interface can be written as

$$\phi^2(\eta)\frac{d\phi(\eta)}{d\eta} \to 0 \quad \text{as} \quad \eta \to \eta_0. \tag{13}$$

This is a very important condition that needs to be imposed when solving the system of equations (12*a–c*). If $d\phi(0)/d\eta$ is less than a certain value, the solutions go to zero at a finite value of η, but only for a certain value of $d\phi(0)/d\eta$ will the solution go to zero while satisfying (13).

In Appendix B it is shown that in order to satisfy (13) it is necessary that $d\phi(\eta_0)/d\eta$ be finite, and, in fact, equal to $-\frac{1}{2}\eta_0$. In order to integrate the equations away from η_0 it is helpful to know the behaviour of the solution near η_0. This allows integration of the equations starting slightly away from the point η_0 where the differential equation is singular. Once it is known that $d\phi(\eta_0)/d\eta$ is finite (12*a*) can be repeatedly differentiated giving

$$\phi(\eta) = -\tfrac{1}{2}\eta_0(\eta-\eta_0) - \tfrac{1}{6}(\eta-\eta_0)^2 - \frac{1}{108\eta_0}(\eta-\eta_0)^3 + O(\eta-\eta_0)^4. \tag{14}$$

Let $\psi(\eta, \xi)$ be the function obtained by integrating (12*a*) backwards from ξ with starting values

$$\psi(\xi,\xi) = 0$$

and

$$\left.\frac{d\psi(\eta,\xi)}{d\eta}\right|_{\eta=\xi} = -\tfrac{1}{2}\xi.$$

In order to find the solution $\phi(\eta)$ an ordinary differential equation solver is used to integrate (12*a*). It can be shown that if $\psi(\eta,\xi)$ is a solution to (12*a*) then so is $f(\eta) = (1/\beta^2)\,\psi(\beta\eta,\xi)$ for any value of β. In order to find the solution, set $\xi = 1$ and integrate (12*a*) backwards from $\eta = 1-\delta\eta$ where $\delta\eta$ is chosen to be a small number and use (14) to find the initial conditions at $\eta = 1-\delta\eta$. By integrating these equations backwards $\psi(0,1)$ can be found. By setting $\beta = (\psi(0,1))^{1/2}$ it is found that $\phi(\eta) = (1/\beta^2)\,\psi(\beta\eta, 1)$ satisfies all of the necessary conditions. It follows that $\eta_0 = 1/(\psi(0,1))^{1/2}$. Finally, the parameter $\delta\eta$ is adjusted so that decreasing it further does not affect the results. The result of this procedure yields

$$\eta_0 = 1.702.$$

Figure 2(*a*) shows a plot of the function $\phi(\eta)$. This problem can be generalized if it is assumed that the groove is initially filled to a height $h_1 = \epsilon h_0$. In this case (12*a, b*) are solved but (12*c*) is replaced by the boundary condition

$$\phi(\eta) \to \epsilon \quad \text{as} \quad \eta \to \infty. \tag{15}$$

When ϵ is non-zero the solutions gradually approach their asymptotic value. Figure 2(*b*) shows plots of the functions $\phi(\eta)$ obtained for different values of ϵ. Note that when ϵ is small the solutions still have continuous first derivatives, but they are approaching the solution for $\epsilon = 0$ which has a discontinuity in its derivative.

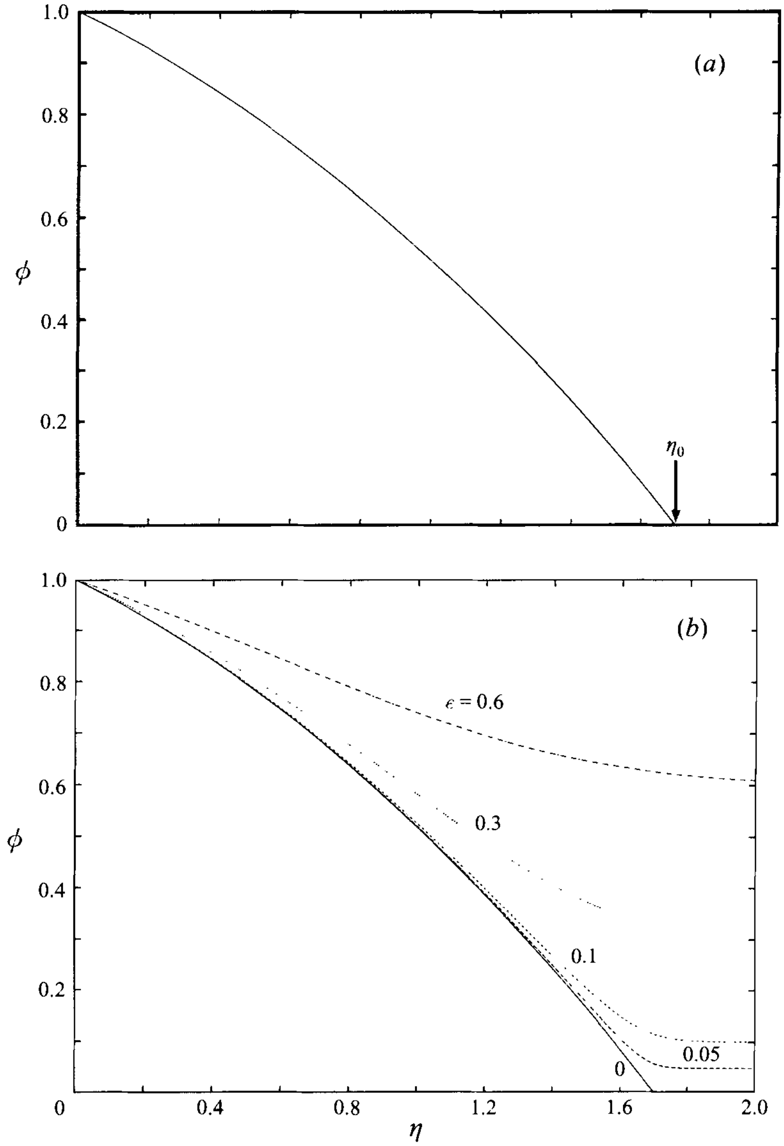

FIGURE 2. The shape function $\phi(\eta)$ plotted versus η: (a) illustrating the definition of the wetting front as η_0; (b) for a partially filled groove.

4. The full similarity solution

A similarity solution is now presented that takes into account the region near the drop where the groove is completely filled with liquid. The assumption that the drop is much larger than the groove disallows a region where θ is significantly larger than α. At any point where $\theta > \alpha$ the capillary pressure is larger than atmospheric pressure. If the radius of the drop is much larger than the height of the groove, then the pressure at such a cross-section would have to be much larger than the pressure in the drop. This would cause the fluid to flow back toward the drop rather than into the groove. Similarly, if the angle θ were significantly smaller than α near the drop, this would cause a very low-pressure region that would cause fluid to rapidly flow into the groove. It follows that near the drop it should be expected that $\theta \approx \alpha$.

A solution will now be found such that for $z < z_1(t)$ the groove is completely filled with fluid, and for $z > z_1(t)$ the groove is only partially filled with fluid. For $z < z_1(t)$, $h(z,t) = h_0$ and $\theta(z,t)$ must satisfy

$$\frac{\partial \hat{A}(\theta(z,t))}{\partial t} = D^* \frac{\partial}{\partial z}\left\{\Gamma(\theta(z,t),\alpha)\cos(\alpha-\theta(z,t))\frac{\partial \theta(z,t)}{\partial z}\right\}. \tag{16}$$

For $z > z_1(t)$, $\theta(z,t) = \theta_0$ and the height $h(z,t)$ must satisfy

$$\frac{\partial h^2(z,t)}{\partial t} = \frac{D}{h_0}\frac{\partial}{\partial z}\left\{h^2(x,t)\frac{\partial h(z,t)}{\partial z}\right\}. \tag{17}$$

At $z = z_1(t)$ the pressure must be continuous which requires that

$$h(z_1(t),t) = h_0, \quad \text{and} \quad \theta(z_1(t),t) = \theta_0. \tag{18a, b}$$

At the interface between the two regions the flux must also be continuous and for this to be true the pressure gradient must be continuous. It follows that

$$\frac{1}{h(z,t)}\frac{\partial h(z,t)}{\partial z} = \cot(\alpha-\theta(z,t))\frac{\partial \theta(z,t)}{\partial z} \quad \text{at} \quad z = z_1(t). \tag{19}$$

As in §3 it is required that the total amount of fluid in the groove be finite for any finite time which requires that

$$\int_{z_1(t)}^{\infty} h^2(z,t)\,\mathrm{d}z < \infty. \tag{20}$$

If the drop is placed on the groove at $t = 0$ this gives the initial conditions

$$z_1(0) = 0, \quad h(z,0) = 0. \tag{21a, b}$$

As in §3 these equations are all invariant under the transformation $t \to \lambda^2 t$ and $z \to \lambda z$. This implies that these equations possess a solution of the form

$$\theta(z,t) = \theta(\eta), \quad h(z,t) = h_0\,\phi(\eta), \tag{22a, b}$$

$$\eta = \frac{z}{(Dt)^{1/2}}, \quad z_1(t) = \eta_1 (Dt)^{1/2}. \tag{22c, d}$$

As $\eta \to \infty$ the same equations obtain as in the last section. The same arguments can be used to show that $\phi(\eta)$ cannot approach zero gradually, but instead must become zero at some finite value η_0 and stay zero for $\eta > \eta_0$. The sidewalls of the groove will not be wet at all for $\eta > \eta_0$, and there will be a pinned region for $\eta < \delta\eta_0 = \eta_1$, where $0 < \delta < 1$ is a constant that needs to be determined as part of the solution process. Depending on whether or not the groove is completely filled the equations are

$$-\tfrac{1}{2}\eta\frac{\mathrm{d}\hat{A}(\theta(\eta),\alpha)}{\mathrm{d}\eta} = \frac{D^*}{D}\frac{\mathrm{d}}{\mathrm{d}\eta}(\Gamma(\theta(\eta),\alpha)\cos(\alpha-\theta(\eta))\frac{\mathrm{d}\theta(\eta)}{\mathrm{d}\eta} \quad \text{for} \quad \eta < \delta\eta_0 \tag{23a}$$

or

$$-\tfrac{1}{2}\eta\frac{\mathrm{d}\phi^2}{\mathrm{d}\eta} = \frac{\mathrm{d}}{\mathrm{d}\eta}\left(\phi^2\frac{\mathrm{d}\phi}{\mathrm{d}\eta}\right) \quad \text{for} \quad \eta > \delta\eta_2. \tag{23b}$$

At $\eta = \delta\eta_0$ the conditions that require continuity of pressure and flux of liquid are

$$\theta(\delta\eta_0) = \theta_0, \quad \phi(\delta\eta_0) = 1 \tag{24a, b}$$

$$\frac{\mathrm{d}\phi}{\mathrm{d}\eta} = \cot(\alpha-\theta_0)\frac{\mathrm{d}\theta}{\mathrm{d}\eta}. \tag{24c}$$

At the point η_0 the dimensionless height ϕ must go to zero:

$$\phi(\eta_0) = 0. \tag{25a}$$

As in the last section the dimensionless flux must also vanish at η_0. This implies the condition

$$\frac{d\phi(\eta_0)}{d\eta} = -\tfrac{1}{2}\eta_0. \tag{25b}$$

and the condition near the drop requires

$$\theta(0) = \alpha. \tag{26}$$

Solutions can be found to the system of equations (23*a*, *b*), (234), (25*a*, *b*), and (26) by Newton's method along with standard ordinary differential equation solvers. By using the similarity property of (23*b*) this problem can be reduced to determining the parameter δ. To do this consider the function $\psi(\eta, \xi)$ that satisfies (23*b*) and the boundary conditions in (25*a*, *b*). The function $\psi(\delta, 1)$ can be determined by solving these equations when $\xi = 1$. As in the previous section the function

$$\phi(\eta, \delta) = \frac{1}{\beta^2}\psi(\beta\eta, 1)$$

also satisfies (23*b*). If $\beta = (\psi(\delta, 1)^{1/2}$ it can be shown that $\phi(\eta, \delta)$ satisfies $\phi(\delta\eta_0(\delta), \delta) = 1$, $\phi(\eta_0(\delta), \delta) = 0$ at $\eta = \eta_0(\delta) = 1/\beta$, and

$$\frac{d}{d\eta}\phi(\eta_0(\delta), \delta) = -\tfrac{1}{2}\eta_0(\delta).$$

Once $\eta_0(\delta)$ is determined, (24) can be used to determine both $\theta(\delta\eta_0(\delta))$ and $(d/d\eta)\,\theta(\delta\eta_0(\delta))$. Once these are determined (23*a*) is integrated from $\eta = \delta\eta_0(\delta)$ to $\eta = 0$ to find $\theta(0, \delta)$. The parameter δ must now be adjusted so that $\theta(0, \delta) = \alpha$.

In order to integrate (23*a*), the functions $\Gamma(\theta, \alpha)$ and $(d/d\theta)\,\Gamma(\theta, \alpha)$ must be evaluated at each step of the solution to the ordinary differential equation. Every evaluation of $\Gamma(\theta, \alpha)$ requires the solution of Poisson's equation on the region of interest. This is by no means an insurmountable computing problem, but it was decided to simplify this part of the calculation by using the approximations in (7*a*) and (7*c*). As already mentioned, these correlations predict $\Gamma(\theta, \alpha)$ to within 2.5% for all values of θ and α such that $\alpha > \theta$. With this in mind (23*a*) is replaced by

$$-\tfrac{1}{2}\eta\frac{d\hat{A}(\theta(\eta), \alpha)}{d\eta} = \frac{\hat{A}^{1/2}(\theta_0, \alpha)}{\sin(\alpha-\theta_0)\,h_0^3(\theta_0, \alpha)}\frac{dG(\theta(\eta), \alpha)}{d\eta}, \tag{27}$$

where

$$G(\eta(\eta), \alpha) = \cos(\theta(\eta)-\alpha)\,h_0^3(\theta(\eta), \alpha)\,\hat{A}^{1/2}(\theta(\eta), \alpha)\frac{d\theta}{d\eta}.$$

Note that in the last section the value η_0 was independent of the parameters θ_0 and α. This is not the case for the solutions described in this section. However, these equations can be solved approximately when $\theta_0 \approx \alpha$ to give a solution that does not depend on either α or θ_0. This solution will now be presented.

It is clear that when $\theta_0 \approx \alpha$ (27) requires that $d\theta(\eta)/d\eta$ be nearly constant. Equation (24) can be approximated by

$$\frac{d\theta(\delta\eta_0)}{d\eta} \approx (\alpha-\theta_0)\frac{d\phi(\delta\eta_0)}{d\eta}. \tag{28}$$

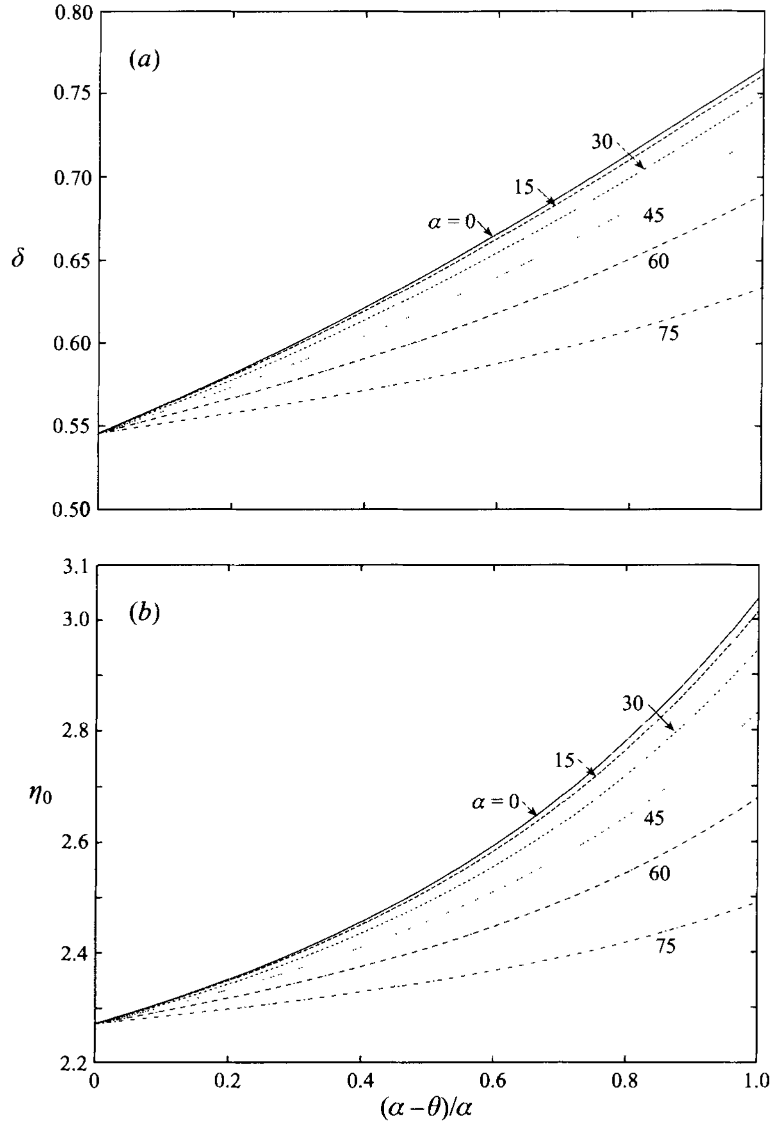

FIGURE 3. The functions (*a*) $\delta(\theta_0, \alpha)$ and (*b*) $\eta_0(\theta_0, \alpha)$, plotted versus $(\alpha-\theta)/\alpha$ for different values of α.

Using the fact that $\mathrm{d}\theta/\mathrm{d}\eta$ is nearly constant on the interval $[0, \delta\eta_0]$ and in order that $\theta(0) = \alpha$ and $\theta(\delta\eta_0) = \theta_0$ the following must be true:

$$\delta\eta_0 \frac{\mathrm{d}\theta(\eta)}{\mathrm{d}\eta} = -(\alpha-\theta_0). \tag{29}$$

When this is combined with the approximate boundary condition in (28) it is found that

$$\delta\eta_0 \frac{\mathrm{d}\phi(\delta\eta_0)}{\mathrm{d}\eta} + 1 = 0. \tag{30}$$

Equation (30) along with the differential equation (23*b*) and the boundary conditions

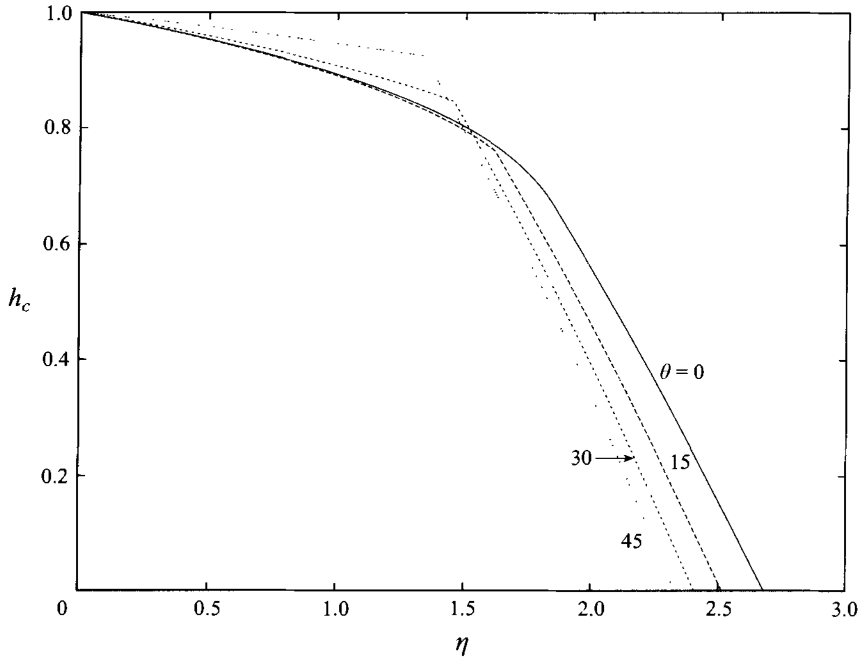

FIGURE 4. The dimensionless height at the centreline of the groove for $\alpha = 60°$ and different values of θ_0.

(25*a*, *b*) can be used to determine the constants δ, η_0 and the function ϕ. This system of equations has been solved numerically using Newton's method. It is found that $\delta = 0.546$ and $\eta_0 = 2.272$.

As in the last section this solution has the advantage that it is not dependent on the parameters θ_0 and α. Note that a considerable fraction of the wetted section of the groove has the fluid pinned to the sidewalls. This contradicts the assumption made in the last section, and as will be shown, is in much better agreement with the results obtained by using the full similarity solution. Figure 3(*a*) shows plots of the function $\delta(\theta_0, \alpha)$ and figure 3(*b*) shows plots of the function $\eta_0(\theta_0, \alpha)$ as functions of $(\alpha - \theta)/\alpha$ for different values of α. As $\theta_0 \rightarrow \alpha$ all of the solutions approach the limiting values predicted by the asymptotic result that assumes $\alpha - \theta_0 \ll 1$. Figure 4 shows plots of the dimensionless height at the centreline of the groove for $\alpha = 60°$ and different values of θ_0. In the pinned region this height is given by $\phi(\eta)\, h_c(\theta(\eta), \alpha)/h_0$, and in the unpinned region it is $\phi(\eta)\, h_c(\theta_0, \alpha)/h_0$.

It should be pointed out that the height at the centreline of the groove does not have a continuous first derivative at the transition point between the pinned and unpinned regions, which is clearly in violation of Laplace's equation for the jump in pressure across an interface. It follows that near this point the assumption that the radius of curvature in the axial direction is small compared to the curvature normal to the axis is not correct. However, away from this point the assumption should be valid.

In §6 a similarity solution will be derived for a drop travelling down an arbitrarily shaped groove, in particular grooves that are rounded at the top rather than sharp like those considered above. When the fluid fills such a groove there is always a well-defined contact angle such that there is no pinned region. The height at the midline would always have continuous derivatives. The problem considered thus far can be considered as the limit of a problem where the sidewalls of the groove gradually flatten out.

Note that figures 3(*a*) and 3(*b*) include plots for $\alpha = 0$. These plots were obtained by numerically letting $\alpha \to 0$. It can be shown analytically that there is in fact a well-behaved limit to our equations as $\alpha \to 0$. However, one should not conclude that this limit models the behaviour of a drop spreading on a flat surface. Our equations depend crucially on the assumption that the drop is spreading in an essentially one-dimensional motion down the groove. Our assumptions do not hold until the drop has spread far down the groove compared to both its height and width. Our equations do not model the spreading of the drop in a direction perpendicular to the groove. If we had a very small-angle groove our equations would at best model the long time behaviour of the drop spreading down it.

5. The volume flux

In this section it will be shown that under certain simplifying assumptions the volume flux has the form given in (6). In Appendix A details are given on how the constant $\Gamma(\theta, \alpha)$ is computed numerically. Let L be the characteristic length scale along the axis of the groove. If it is assumed that $h/L \ll 1$ then locally the flow in the groove appears to be independent of z, and the axial contribution to the mean curvature can be ignored. As in Poiseuille flow, it is possible to satisfy the equations of motion by assuming that the velocity field is independent of z and has a component in the z-direction only, and that there is a constant pressure gradient in the z-direction. In a cylindrical coordinate system (r, ϕ, z) the velocity vector and pressure are given by

$$\boldsymbol{u}(r, \phi, z) = (0, 0, w(r, \phi)),$$

$$\frac{\partial p}{\partial z} = \text{constant}.$$

This velocity field automatically satisfies the continuity equation for an incompressible fluid. In order to satisfy the momentum balance in the Navier–Stokes equations w must satisfy

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial w}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 w}{\partial \phi^2} = \lambda, \tag{31a}$$

where

$$\lambda = \frac{1}{\mu}\frac{\partial p}{\partial z}. \tag{31b}$$

Here, the time rate of change of w has been ignored, which is valid provided that

$$\frac{h^2}{T\mu} \ll 1,$$

where T is the characteristic time for the change in the velocity field. From self-similarity $L^2 = DT$, where L is the characteristic length scale. From the definition of D, in order to ignore the time derivatives of w, the inequality $h_0^3 \gamma\rho/(\mu^2 L^2) \ll 1$ must hold.

The no-slip boundary condition gives

$$w(r, \phi) = 0 \quad \text{for} \quad \phi = \pm(\tfrac{1}{2}\pi - \alpha). \tag{32a}$$

The free surface can be written as

$$r(\phi) = h(z, t) f(\phi, \theta_0, \alpha), \tag{32b}$$

where f is chosen so that the curvature of the surface is constant, and the surface meets the wall with a contact angle of θ_0. It is important to emphasize that the free surface scales according to the height $h(z, t)$ at the wall. If it is assumed that the viscosity of the fluid above the liquid surface is negligible, then the surface of the fluid must satisfy the stress-free boundary condition

$$-\boldsymbol{\sigma}\cdot\boldsymbol{n} = \left(-\frac{\gamma}{R}+p_0\right)\boldsymbol{n} \quad \text{on} \quad r(\phi) = h(z,t)f(\phi,\theta_0,\alpha). \tag{32c}$$

Here, $\boldsymbol{\sigma}$ is the stress tensor given by

$$\sigma_{ij} = -p\delta_{ij} + 2\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right), \tag{32d}$$

$\boldsymbol{n}$ is the normal to the surface, and p_0 is the pressure above the liquid surface. It is assumed that there is no axial component to the normal, hence

$$\boldsymbol{n} = (n_r, n_\phi, 0). \tag{32e}$$

The boundary conditions at the free surface can now be written

$$\frac{\partial w}{\partial n} = 0 \quad \text{on} \quad r(\phi) = h(z,t)f(\phi,\theta_0,\alpha), \tag{33a}$$

$$p = -\frac{\gamma}{R}+p_0. \tag{33b}$$

It is clear that if $\psi(r,\phi)$ is a function that satisfies

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} = 1, \tag{34a}$$

$$\psi(r,\theta) = 0 \quad \text{for} \quad \theta = \pm(\tfrac{1}{2}\pi-\alpha), \tag{34b}$$

$$\frac{\partial\psi(r,\phi)}{\partial n} = 0 \quad \text{for} \quad r = f(\phi,\theta_0,\alpha) \tag{34c}$$

then it is possible to write

$$w(r,\phi) = \lambda h^2(z,t)\,\psi\left(\frac{r}{h(z,t)},\phi\right). \tag{35}$$

The volumetric flow rate can be written as

$$q = 2\int_0^{\frac{1}{2}\pi-\alpha}\int_0^{h(z,t)f(\phi,\theta_0,\alpha)} rw(r,\phi)\,\mathrm{d}r\,\mathrm{d}\phi.$$

In terms of the function ψ this can be written as

$$q = -\lambda h^4(z,t)\,\Gamma(\theta_0,\alpha) = -\frac{h^4(z,t)}{\mu}\Gamma(\theta_0,\alpha)\frac{\partial p}{\partial z} \tag{36a}$$

where

$$\Gamma(\theta_0,\alpha) = -2\int_0^{\frac{1}{2}\pi-\alpha}\int_0^{f(\phi,\theta_0,\alpha)} r\psi(r,\phi)\,\mathrm{d}r\,\mathrm{d}\phi. \tag{36b}$$

The function $\Gamma(\theta_0,\alpha)$ needs to be computed numerically. The details of this numerical calculation are given in Appendix A.

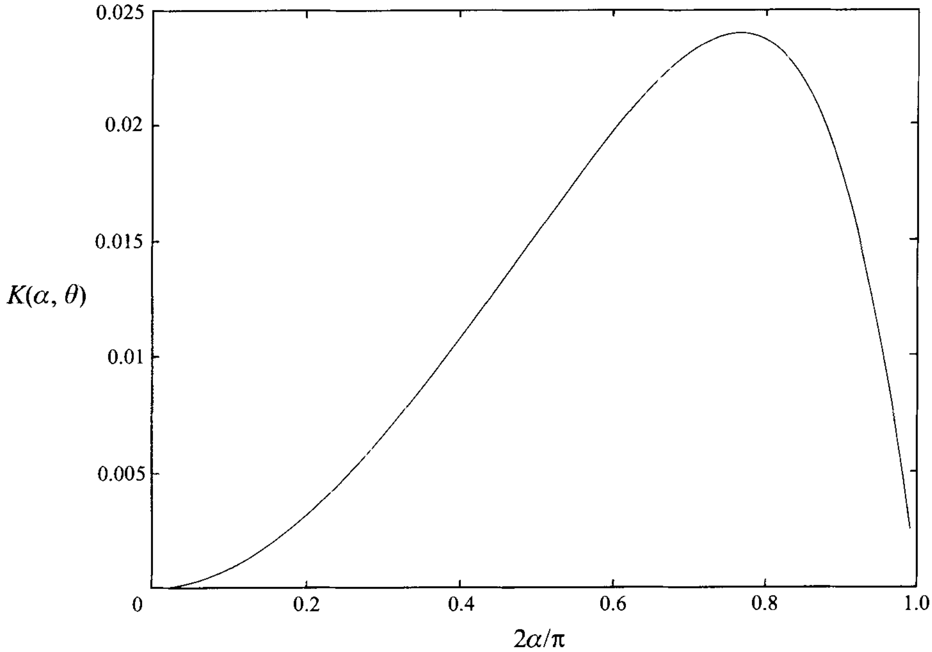

FIGURE 5. The function $K(\alpha, \theta)$ plotted versus α for $\theta = 0°$ that suggests a maximum flow rate at approximately $\alpha = 70°$.

The correlation in (7*a*) was obtained in the following manner. The calculations begin with the expansions

$$\Gamma(\alpha,\alpha) \approx \tfrac{1}{6}\cot^3(\alpha) - \tfrac{1}{2}\cot^5(\alpha) \quad \text{as} \quad \alpha \to \tfrac{1}{2}\pi$$

and

$$\Gamma(\alpha,\alpha) \approx \tfrac{1}{6}\cot(\alpha) - \frac{1}{2\cot(\alpha)} \quad \text{as} \quad \alpha \to 0.$$

These expansions can be derived with the use of straightforward asymptotic methods. Both of these expansions have been verified using the numerical methods described in Appendix A. A rational function approximation to this solution is now sought that has the right asymptotic behaviour in the limiting case described above. The rational function

$$Q_\lambda(\alpha) = \frac{1}{6}\frac{\cot^3(\alpha) + \lambda\cot^4(\alpha) + \cot^5(\alpha)}{1 + \lambda\cot(\alpha) + 4\cot^2(\alpha) + \lambda\cot^3(\alpha) + \cot^4(\alpha)}$$

has the correct behaviour as $\cot(\alpha) \to 0$ and as $\cot(\alpha) \to \infty$ for any value of λ.

The correlation in (7*a*) was obtained by sweeping through α for each value of λ and recording the largest percentage difference between the correlation, and the numerical results. The value of λ was then varied in order to minimize this percentage difference. It was found that $\lambda = 3.4$ gave excellent agreement between this correlation and the numerical results. The error was less than 0.1% for all values of α.

The correlation in (7*c*) was obtained by assuming that $\Gamma(\theta_0, \alpha)$ was proportional to $\Gamma(\alpha, \alpha)$ times the area raised to a power, and h_c raised to a power. These powers were adjusted until the relative error between the numerical results and the correlation was less than 2.5%.

The function $K(\theta_0, \alpha)$ in (8*c*) is the function that gives the effect of the geometry on the diffusion coefficient in (8*b*). Figure 5 shows a plot of this function for $\theta_0 = 0$ and

$0 < \alpha < \frac{1}{2}\pi$. It is interesting to note that this function is not monotonic in α. This means that there is a certain angle for which flow in the groove will be maximal.

6. Arbitrarily shaped grooves

So far the groove of interest has been V-shaped and embedded in an otherwise flat surface. In this section an outline will be given of a similar analysis for an arbitrarily shaped groove with constant cross-section. It will be shown that for such a groove a similarity solution still obtains and the front of the fluid will move like $(Dt)^{1/2}$.

As in the last section it could be assumed that there is a sharp discontinuity in the sidewalls (at the point where the groove intersects the flat surface). Instead, it will be assumed that the sidewalls of the groove smoothly approach the flat surface. In this case there will be a height, h_0, at which the free surface of the filled groove will be flat. For an arbitrarily shaped groove the cross-sectional area is not necessarily proportional to h^2. In general

$$\text{Area} = h_0^2 \hat{A}(\hat{h}, \theta), \tag{37}$$

where $\hat{h} = h/h_0$.

The radius of curvature is no longer proportional to h. In general it is given by

$$\frac{1}{R} = \frac{1}{h_0} \hat{K}(\hat{h}, \theta). \tag{38}$$

It cannot be assumed that the flux is proportional to h^4; instead it is written

$$q = -\frac{1}{\mu} h_0^4 \hat{q}(\hat{h}, \theta) \frac{\partial p}{\partial z}. \tag{39}$$

Use of (1) and (4) yields

$$\frac{\partial \hat{A}(\hat{h}, \theta)}{\partial t} = D \frac{\partial}{\partial z}\left(\hat{q}(\hat{h}, \theta) \frac{\partial \hat{K}}{\partial z}\right), \tag{40}$$

where

$$D = h_0 \gamma / \mu.$$

As with the V-shaped groove, it is required that as the drop is approached, the liquid must be flat which requires that $\hat{h}(0, t) = h_0$. With no fluid in the groove the initial condition becomes $\hat{h}(z, 0) = 0$. No matter how general the function $\hat{q}$, $\hat{K}$, and $\hat{A}$, it can be shown that the system of equations (37)–(40) and (6) are all invariant under the one-parameter group of transformations $t \to \lambda^2 t$ and $z \to \lambda z$. This implies that the equations have solutions of the form

$$\hat{h}(z, t) = \phi(\eta),$$

$$\eta = \frac{z}{(Dt)^{1/2}}.$$

If the groove is wedge shaped as $h \to 0$, the same argument as was used for the V-shaped groove can be used to show that the height must go to zero at a finite value of η. In this case the front of the fluid, once again, can be written as $z_0(t) = \eta_0 (Dt)^{1/2}$. Note that when the sidewalls of the groove are smooth (except at the tip) there is no need to have a pinned region. If we take walls that are smooth and let them approach walls that have an abrupt edge like those in the V-shaped groove, we expect that the solutions will approach those of the V-shaped groove. In particular, when the sidewalls are smooth there is no discontinuity in the interface between the pinned and unpinned regions (since there is no pinned region). It should be noted that the theory gets into trouble if the groove is smooth as $h \to 0$. This case is similar to that of the V-shaped groove where $\theta_0 < \alpha$. In this case $\mathrm{d}\hat{K}/\mathrm{d}\hat{h} > 0$ as $h \to 0$. This gives an equation that behaves like a diffusion equation with negative diffusivity which will lead to an ill-posed mathematical problem. In this case it is argued that it is necessary to include the effect of the surface curvature in the axial direction. This will lead to a term like

$$K = \frac{1}{R(\hat{h}(z))} + \frac{\partial^2 h}{\partial z^2}.$$

With this term, including the second derivative, (40) will involve spatial derivatives of fourth order. This term is always of a sign such that the equations are well posed no matter what the sign of $\mathrm{d}\hat{K}/\mathrm{d}h$.

If the groove does not come to a wedge as $h \to 0$, the drop may or may not flow into it. If the drop does flow into the groove there must be a region where higher-order spacial derivatives must be included in (37). These higher-order spacial derivatives will destroy the self-similarity of the equations. If the groove is nearly V-shaped as $h \to 0$, but is rounded near the tip, the exact self-similarity will be destroyed, but approximate self-similarity will remain.

7. Stability of a filled groove

The diffusion coefficient D in (8*b*) is negative when $\alpha < \theta$. In this section a thermodynamic argument will be given that shows that under this condition, the groove will not be filled with liquid. Note that this condition complements the work by Concus & Finn (1969) who showed that no finite-length equilibrium solution can exist in a V-shaped groove if $\alpha > \theta$. Let σ_{lv}, σ_{ls}, and σ_{sv} be the surface energies between the liquid/vapour, liquid/solid, and solid/vapour, respectively. Here the vapour is assumed to be the atmosphere that fills the groove before the drop is placed on the groove. Assuming that the radius of the drop is much larger than the height of the groove, the groove must be filled so that the free surface of the liquid is almost completely flat. If this is true the change in the total surface energy per unit distance caused by flow into the groove is given by

$$\Delta E = 2(\sigma_{ls} - \sigma_{sv}) \frac{h_0}{\sin(\alpha)} + 2h_0 \cot(\alpha)\, \sigma_{lv}.$$

It is justifiable to ignore the change in surface energy of the drop provided the radius of the drop is much larger than the height of the groove. Now, the total surface energy per unit distance decreases provided

$$\frac{\sigma_{ls} - \sigma_{sv}}{\sigma_{lv}} + \cos(\alpha) > 0$$

or expressed alternatively

$$\cos(\alpha) - \cos(\theta_0) < 0. \tag{41}$$

Keeping in mind the geometrical constraint that $0 < \alpha < \frac{1}{2}\pi$, (41) will be true provided that $\alpha > \theta_0$. It can be seen that the diffusion coefficient is positive if and only if it is thermodynamically favourable to fill the groove with liquid. This thermodynamic criterion can be used to show how imperfections in the groove affect whether or not it will fill up with liquid. As an example, suppose the bottom of the groove is flattened so that it does not come to a sharp point. In particular, suppose that the surface of the groove is given by

$$y = \tan(\alpha)x \quad \text{for} \quad \epsilon h_0 \cot(\alpha) < |x| < h_0 \cot(\alpha)$$

and $$y = \epsilon h_0 \quad \text{for} \quad 0 < |x| < \epsilon h_0 \cot(\alpha).$$

In this case the difference in total surface energy per unit distance, before and after the groove is filled, is given by

$$\Delta E = 2h_0(\sigma_{ls} - \sigma_{sv})\left(\frac{1-\epsilon}{\sin(\alpha)} + \epsilon \cot(\alpha)\right) + 2h_0 \cot(\alpha)\, \sigma_{lv}.$$

The total surface energy decreases provided

$$\cos(\alpha) < \left(\frac{1-\epsilon}{1-\epsilon\cos(\theta_0)}\right)\cos(\theta_0).$$

The fact that

$$\frac{1-\epsilon}{1-\epsilon\cos(\theta_0)} < 1$$

shows that when ϵ is non-zero, α must be larger than when $\epsilon = 0$ in order for the groove to be filled with liquid.

8. Conclusions

Equations for the capillary flow kinetics of a liquid in a V-shaped groove have been derived. With most assumptions regarding the scale of the groove dimensions, the resulting mean curvature, and an appropriate expression for mass conservation, a partial differential equation was developed for the shape of the liquid filling the groove. This equation was shown to be a nonlinear diffusion equation having a similarity solution which suggested that the liquid wetting front moved as $(Dt)^{1/2}$ where D is the diffusion coefficient. It was shown that for a well-posed problem the diffusion coefficient must be positive which implied that the basal groove angle relative to the horizontal must be greater than the contact angle between the liquid and the groove surface. This same condition for flow in a V-shaped groove was shown to obtain from a purely thermodynamic argument thus demonstrating self-consistency between the kinetic flow model and equilibrium reasoning. It was also demonstrated that many grooves of arbitrary shape will exhibit the same $(Dt)^{1/2}$ flow kinetics since the flow equations for these grooves remain invariant under the similarity transform used for V grooves. Certain groove shapes do not lead to these simple flow kinetics and it is recommended that liquid surface curvature along the length of the groove be included in the model.

The following is a list of our main results that can be directly compared to experiments:

(i) For a V-shaped groove the position of the leading edge of the fluid can be written as:

$$z_0(t) = \eta_0(\theta_0, \alpha)(Dt)^{1/2} \quad \text{where} \quad D = (\gamma h_0/\mu)^{1/2} K(\theta_0, \alpha).$$

(ii) The diffusivity D will be negative unless $\alpha > \theta_0$. If the diffusivity is negative it is not energetically favourable for the drop to spread down the groove.

(iii) When $\alpha = \theta_0$ is small we have $\eta_0 \approx 2.272$. When $\alpha - \theta_0$ is not small the value of η_0 can be increased by as much as 40%. Figure 3(*b*) shows plots of the function $\eta_0(\theta_0, \alpha)$ for different values of α.

(iv) The free surface of the liquid spreading down the groove should be self-similar. In particular, if $z_0(t)$ is the leading edge of the fluid, then the groove will be completely filled for $x < z_1(t) = \delta(\theta_0, \alpha) z_0(t)$. For $\alpha - \theta_0$ small, we have $\delta_0 \approx 0.546$. Figure 3(*a*) shows plots of $\delta(\theta_0, \alpha)$ for different values of α. When $\alpha - \theta_0$ is not small, $\delta(\theta_0, \alpha)$ can be as large as 0.75.

(v) The function $K(\theta_0, \alpha)$ gives the dependence of D on the geometry of our system. An approximate analytical expression for $K(\theta_0, \alpha)$ can be found by substituting into equations (5*b*), (7*a*–*c*), and (8*c*). It is interesting to note that $K(\theta_0, \alpha)$ is not a monotonic function of the angle α. There is a maximum value of α that maximizes $K(\theta_0, \alpha)$ and hence the spread of the drop down the groove.

The authors would like to thank J. A. Mann and R. R. Rye for their helpful discussions on capillary-driven flow in grooves. This work was performed at Sandia National Laboratories, which is supported by the Department of Energy under contract number DE-AC04-94AL85000.

Appendix A. Evaluation of the function $\Gamma(\theta, \alpha)$

In this Appendix details are given of the numerical computation of the function $\psi(r, \phi)$ that satisfies (34), and the computation of the function $\Gamma(\theta, \alpha)$ in (36*b*). First, the function $f(\phi, \theta, \alpha)$ that gives the shape of the free surface will be calculated. Henceforth, the functional dependence on the parameters θ and α will be dropped when referring to the function f. Discussion will be limited to the case $\alpha > \theta$ since this gives a positive diffusion coefficient. With reference to figure 1(*b*) note that the radius of curvature of the interface is given by

$$\frac{1}{R(\theta, \alpha)} = \frac{\sin(\alpha - \theta)\tan(\alpha)}{h(z, t)}.$$

The centre of curvature is a distance x_0 above the apex of the groove. From figure 2 it can be seen that $x_0 = 1 + \cot(\alpha - \theta)\cot(\alpha)$. On the free surface

$$(x - x_0)^2 + y^2 = R^2,$$

and if $(x, y) = f(\phi)(\cos(\phi), \sin(\phi))$ then it is found that

$$f(\phi) = x_0 \cos(\phi) - [R^2 - x_0^2(\theta, \alpha)\sin^2(\phi)]^{1/2}.$$

The normal to the surface is given by

$$\boldsymbol{n} = \frac{f\boldsymbol{e}_r - f_\phi \boldsymbol{e}_\phi}{(f^2 + f_\phi^2)^{1/2}}.$$

Here $\boldsymbol{e}_r$ and $\boldsymbol{e}_\phi$ are the unit normals in cylindrical coordinates. Use is made of the fact that an inhomogeneous solution to (34) is

$$\psi^*(r, \phi) = \frac{r^2}{4}\left(1 - \frac{\cos(2\phi)}{\cos(2(\frac{1}{2}\pi - \alpha))}\right).$$

This yields

$$\psi(r, \phi) = \psi_h(r, \phi) + \psi^*(r, \phi),$$

where

$$\nabla^2 \psi_h = 0, \tag{A 1}$$

$$\psi_h(r, \phi) = 0 \quad \text{for} \quad \phi = \pm(\tfrac{1}{2}\pi - \alpha), \tag{A 2}$$

$$\frac{\partial \psi_h}{\partial n} = -\frac{\partial \psi^*}{\partial n} = \hat{g}(\phi). \tag{A 3}$$

The solution ψ_h is the function that minimizes the functional

$$\Lambda(w) = \frac{1}{2}\int_V |\nabla w|^2 \,\mathrm{d}v - \int_s g w \,\mathrm{d}s \tag{A 4}$$

subject to the constraint that

$$w(r,\phi) = 0 \quad \text{for} \quad \phi = \tfrac{1}{2}\pi - \alpha. \tag{A 5}$$

In (A 4) the first term is integrated over the volume of fluid, and the second is integrated over the free surface. An approximate solution is now found by writing ψ_h as a finite sum that automatically satisfies the boundary conditions at $\phi = \pm(\frac{1}{2}\pi - \alpha)$ and that satisfies Laplace's equation

$$\psi_h(r,\phi) = \sum_{k=0}^{N} a_k \psi_k(r,\phi), \tag{A 6}$$

$$\psi_k(r,\phi) = r^{\lambda_k}\cos(\lambda_k \phi), \tag{A 7}$$

$$\lambda_k = \frac{\frac{1}{2}\pi + k\pi}{\frac{1}{2}\pi - \alpha}. \tag{A 8}$$

For any set of coefficients a_k the functional can be written as

$$\Lambda(\boldsymbol{a}) = \frac{1}{2}\sum_{i=0}^{N}\sum_{j=0}^{N} A_{ij} a_i a_j - \sum_{k=0}^{N} a_k b_k,$$

where
$$b_k = 2\int_0^{\pi/2-\alpha} f^{\lambda_k}(\phi)\cos(\lambda_k\phi)\,\hat{g}(\phi)\,(f^2 + f_\phi^2)^{1/2}\,\mathrm{d}\phi$$

and
$$A_{ij} = \int_V \nabla\psi_i \cdot \nabla\psi_j \,\mathrm{d}v = 2\frac{\lambda_i \lambda_j}{\lambda_i + \lambda_j}\int_0^{\pi/2-\alpha} f^{\lambda_i+\lambda_j}(\phi)\cos((\lambda_i - \lambda_j)\phi)\,\mathrm{d}\phi.$$

The coefficients A_{ij} and b_{ij} are obtained with use of numerical quadrature. An approximation to the function ψ_h is obtained by fixing N and minimizing $\Lambda(\boldsymbol{a})$. This leads to a linear system of equations for the coefficients a_k that can be solved numerically. Once the coefficients are known, it remains to determine the quantity Γ which can be written as

$$\Gamma(\theta,\alpha) = 2\int_0^{\pi/2-\alpha}\int_0^{f(\phi)} r\left(\psi^*(r,\phi) + \sum_{k=0}^{N} a_k r^{\lambda_k}\cos(\lambda_k\phi)\right)\mathrm{d}r\,\mathrm{d}\phi.$$

A simple calculation shows that this can also be written as

$$\Gamma(\theta,\alpha) = \beta^* + \sum_{k=0}^{N}\alpha_k\beta_k, \tag{A 9}$$

where
$$\beta^* = \frac{1}{8}\int_0^{\pi/2-\alpha} f^4(\phi)\left(1 - \frac{\cos(2\phi)}{\cos(2(\frac{1}{2}\pi - \alpha))}\right)\mathrm{d}\phi \tag{A 10}$$

and
$$\beta_k = \frac{2}{\lambda_k + 2}\int_0^{\pi/2-\alpha} f^{\lambda_k+2}(\phi)\cos(\lambda_k\phi)\,\mathrm{d}\phi. \tag{A 11}$$

Appendix B. Certain proofs regarding the function $\phi(\eta)$

In this Appendix several results are proven concerning the system of equations (12*a–c*). First it is proven that no solution to this system of equations can approach zero gradually as $\eta \to \infty$. To show this (12*a*) is integrated from η to η^* to get

$$\phi^2(\xi)\left(\frac{d\phi(\xi)}{d\eta}+\tfrac{1}{2}\xi\right)\Bigg|_{\eta}^{\eta^*} = \frac{1}{2}\int_{\eta}^{\eta^*} \phi^2(\xi)\,d\xi. \tag{B 1}$$

Now the behaviour of (B 1) is examined as $\eta^* \to \infty$. In order to satisfy (12*c*) it is necessary that $\phi^2(\eta)\,\eta \to 0$ as $\eta \to \infty$. It follows that

$$\phi^2(\eta)\left(\frac{d\phi(\eta)}{d\eta}+\tfrac{1}{2}\eta\right) \leqslant 0 \quad \forall\, \eta. \tag{B 2}$$

It is now clear that as $\eta \to \infty$ it is necessary that $\phi(\eta) \equiv 0$. If this were not the case then it would be necessary that

$$\phi^2(\eta)\left(\frac{d\phi(\eta)}{d\eta}+\tfrac{1}{2}\eta\right) \leqslant 0 \quad \text{as} \quad \eta \to \infty.$$

This is not possible since this would imply that the function $\phi(\eta)$ did not approach zero as $\eta \to \infty$. It is concluded that it is necessary to have the function $\phi(\eta)$ go to zero at some point $\eta = \eta_0$. Note that (B 1) also implies that $\phi(\eta)$ must be a monotonically decreasing function outside the region where $\phi(\eta) \equiv 0$. It will now be shown that in order to satisfy (13) it is necessary that $d\phi(\eta_0)/d\eta$ is finite. This follows with use of (B 1) with $\eta^* = \eta_0$. In this case it is found that

$$\phi^2(\eta)\left(\frac{d\phi(\eta)}{d\eta}+\tfrac{1}{2}\eta\right) = \frac{1}{2}\int_{\eta_0}^{\eta} \phi^2(s)\,ds = \phi^2(\eta) f(\eta).$$

Here $f(\eta)$ is a function that, owing to the monotonicity of $\phi(\eta)$, can be shown to satisfy

$$f(\eta) = o(1) \quad \text{as} \quad \eta \to \eta_0,$$

and it follows that

$$\frac{d\phi(\eta)}{d\eta}+\tfrac{1}{2}\eta - f(\eta) = 0.$$

It is clear that $d\phi(\eta)/d\eta$ must remain finite as $\eta \to \eta_0$, and in fact

$$\frac{d\phi(\eta_0)}{d\eta} = -\tfrac{1}{2}\eta_0. \tag{B 3}$$

REFERENCES

ADAMS, C. M. 1966 Spreading, penetration, and capillary flow in metallic systems. In *Fundamental Phenomena in the Materials Sciences*, Vol. 2 (ed. L. J. Bonis & H. H. Hausner), p. 175. Plenum.

BASCOM, W. D., COTTINGTON, R. L. & SINGLETERRY, C. R. 1964 Dynamic surface phenomena in the spontaneous spreading of oils on solids. In *Contact Angle, Wettability, and Adhesion* (ed. R. F. Gould), p. 355. American Chemical Society.

BELL, J. M. & CAMERON, F. K. 1906 Movement of liquids through capillary tubes. *J. Phys. Chem.* **10**, 658.

CONCUS, P. & FINN, R. 1969 On the behavior of a capillary surface in a wedge. *Proc. Natl Acad. Sci.* **63**, 292.

COTTINGTON, R. L., MURPHY, C. M. & SINGLETERRY, C. R. 1964 Effect of polar-nonpolar additives on oil spreading on solids, with applications to nonspreading oils. In *Contact Angle, Wettability, and Adhesion* (ed. R. F. Gould), p. 341. American Chemical Society.

LENORMAND, R. & ZARCONE, C. 1984 Role of roughness and edges during imbibation in square capillaries. In *59th Annual Technical Conference and Exhibition. Society of Petroleum Engineering.*

PARKER, E. R. & SMOLUCHOWSKI, R. 1944 Capillarity of metallic surfaces. *Trans. ASME* **35**, 362.

SHEPARD, J. W. & BARTELL, F. E. 1953 Surface roughness as related to hysterisis of contact angles. III. *J. Phys. Chem.* **57**, 458.

SHUTTLEWORTH, R. & BAILEY, G. L. J. 1948 The spreading of a liquid over a rough solid. *Disc. Farad. Soc.* **3**, 16.

WASHBURN, E. W. 1921 The dynamics of capillary flow. *Phys. Rev.* **17**, 273.