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Abstract

We study numerical solutions to the equation of capillary surfaces in trapezoidal domains when the boundary contact angle declines from 90^{o} to some critical value. There is also obtained a result on behavior of solutions in more general domains that confirms numerical calculations.

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0. Introduction

In this paper we study the behavior of numerical solutions to the capillary problem in the absence of gravity for a cylindrical capillary tube with trapezoidal cross-section.

From the mathematical point of view the physical properties of a liquid in a capillary tube in the absence of gravity can be described with the help of only one parameter -- the contact angle. This is the angle between the capillary surface and the walls of the cylinder. For homogeneous material of walls, the contact angle must be constant along the boundary.

P. Concus and R. Finn [1] have shown that the capillary surface does not exist for all physically reasonable contact angles. They obtained a necessary condition for existence of the solution. The condition gives an estimate of the contact angle in terms of geometry of the base domain of the cylinder. In the case that gravity is absent the estimate is essentially non-local, as it can not be expressed by means of local geometrical characteristics of the boundary.

R. Finn in [2] noticed that even for a polygonal domain one cannot infer information on the existence of a solution from knowledge of the vertex angles alone. He has shown that a trapezoidal domain presents a good example in the sense that for any γ_0, $0 < \gamma_0 < \pi/2$, there exists a small deformation of rectangular domain to a trapezoidal one such that there is

no solution in the trapezoidal domain for contact angles less than γ_0. For the rectangular domain a solution exists for any angle larger than $\pi/4$.

We will describe the results of two kinds of numerical experiments. First, for a fixed trapezoid, we consider solutions as the contact angle declines from $\pi/2$ to some apparently critical angle; and second we consider the behavior of solutions as the base domain is deformed from a rectangle to some critical trapezoid (with the contact angle fixed).

1. Capillarity phenomena

We adduce here some information on capillarity phenomena. For a detailed presentation we refer to the article of R. Finn [3].

We consider a liquid partly filling a vertical cylinder with a base domain Ω; the boundary of Ω is denoted by Σ. We assume that the height of the equilibrium free surface of the liquid in the cylinder is a single-valued smooth function $u(x,y)$. We assume also that the volume of the liquid is sufficiently large to cover the base of the cylinder entirely.

In the absence of gravity the height $u(x,y)$ of the liquid over the bottom of the cylinder satisfies the equation

$$\operatorname{div}\left(\frac{1}{W}\nabla u\right) = 2H \tag{1}$$

where $\nabla u = (\partial u/\partial x, \partial u/\partial y)$, $W = (1 + |\nabla u|^2)^{1/2}$.

The constant H is the mean curvature of the liquid surface. It is defined by the cross-sectional shape of the cylinder and the boundary con-

dition satisfied by the free surface of the liquid at the cylinder wall.

We will demand the free surface make a prescribed contact angle γ with the cylinder wall. Thus the boundary condition is

$$\frac{1}{W}\frac{\partial u}{\partial n} = \cos\gamma \tag{2}$$

for $(x,y) \in \Sigma$. Here $\partial u/\partial n$ is the derivative with respect to the outward directed normal at the wall.

To the equation in divergence form (1) with boundary condition (2) there corresponds the following variational principle. The solution of (1),(2) is the minimum of the energy functional

$$E(u) = \int_{\Omega} W\,dxdy + 2H\int_{\Omega} u\,dxdy - \cos\gamma \int_{\Sigma} u\,d\sigma \ . \tag{3}$$

Eq. (1) is the Euler equation for the variational problem of minimizing (3).

Applying the divergence theorem to (1) with boundary condition (2) we obtain the relation between the mean curvature and the contact angle:

$$2H\Omega = \Sigma\cos\gamma \tag{4}$$

Here and also later we use the same symbols to denote domains and their measures. Eq. (4) is a necessary condition for existence of the solution to (1),(2). P. Concus and R. Finn in [1] obtained in addition a more general condition than (4).

Let the cross-section Ω of the cylinder be cut into two parts Ω^* and $\Omega\backslash\Omega^*$ by a curve Γ, which intersects the boundary Σ at points p_1 and p_2. Let Σ^* denote the part of Σ cut off by Γ and adjacent to

Ω^*. Applying the divergence theorem to the domain Ω^* and taking into account that $|\nabla u/W| \leq 1$ along Γ (as everywhere), Concus and Finn proved the estimate

$$\cos \gamma \leq V \tag{5}$$

where

$$V = \min \frac{\Gamma/\Sigma}{|\Sigma^*/\Sigma - \Omega^*/\Omega|} \tag{6}$$

The minimization is carried over all curves Γ described above such that $\Sigma^*/\Sigma - \Omega^*/\Omega$ is nonzero. The estimate (5) holds if the solution to (1) and (2) exists.

2. Symmetry of the solution

In our calculations for a trapezoidal domain we will employ the following simple property of the capillary problem.

Theorem: Let $u(x,y)$ be a solution to the problem (1) and (2) in a domain Ω that is invariant under reflection: $x' = -x$, $y' = y$. Then $u(x,y)$ is also symmetric

$$u(x,y) = u(-x,y) \quad .$$

Proof: We put

$$v(x,y) = u(x',y') \equiv u(-x,y) \quad .$$

It is easy to see that the equation (1) and the boundary condition (2) are also invariant under reflection. Thus $v(x,y)$ has to be a solution to (1) and (2), and by virtue of the uniqueness

$$v(x,y) \equiv u(x,y) \quad .$$

(A uniqueness theorem for (1) and (2) is straightforward, following immediately from the variational formulation of the problem, since the energy functional (3) is convex.)

Remark: The theorem is true for any domain, invariant under orthogonal transformation, say for a regular polygon.

3. Computational experiments

Now we consider the problem (1) and (2) when the base domain is a trapezoid.

For numerical experiments an equilateral trapezoid was chosen with the following parameters: the long base $b = 2.$, the short base $a = 1.3$ and the height $h = 25.$ The angles of the trapezoid are very close to 90°, approximately $90^{\circ} \pm 0.8^{\circ}$. This trapezoid has sufficiently large altitude to exhibit clearly the nonexistence phenomenon under study, but not so large as to require an excessive number of mesh points for representation of the solution. The departure from a rectangle is sufficient to permit visualization of the change to the trapezoid when the shorter base is decreased from 2 to 1.3.

For the trapezoid the quantity V in (5) giving an upper bound for the cosine of the contact angle can be calculated numerically. The minimum

of the expression (6) for V is realized when Γ is a particular circular arc connecting sides of the trapezoid. The calculations gave for the critical angle γ_0 for the trapezoid with the above parameters an approximate value

$$\gamma_0 \doteq 57.6^\circ$$

In view of the theorem we solve Eq. (1) in the half-trapezoid

$$T = \{(x,y) \mid 0 \leq y \leq 25, \quad 0 \leq x \leq 1 - 0.014y\}$$

with the boundary condition (2) on the half-perimeter of the trapezoid and the boundary condition

$$\partial u/\partial n \mid_{x=0} = 0 \quad .$$

The problem was solved numerically using a suitably modified version of R. A. Brown's finite-element program [4] for the capillary problem in a rectangle. The domain was discretized employing a trapezoidal grid constructed as follows. Each base of the half trapezoid T was divided equidistantly into M parts and the height was divided equidistantly into N parts. Mesh points were formed by intersections of the mesh lines connecting the obtained points on the bases and the mesh lines parallel to the x-axis through the points of partition of the height.

The program used reduced quadratic polynomials as the basis functions for the finite-element method (the reduced quadratic element differs from the full biquadratic element by the elimination of the x^2y^2 term and omissions of the centroid node). The resulting non-linear algebraic prob-

lem is solved using Newton's method.

Computations were carried out with $N = 50$, $M = 4$, and were repeated for $N = 75$, $M = 7$. The two series of computations showed very good consistency between their results. The method was tested for the 2 x 25 rectangle for contact angles close to 45°. The method converged for $\gamma \geq 46^\circ$ and did not converge for $\gamma \leq 45^\circ$ (the step of changing the contact angle in test calculations was 1°).

The results are depicted in figures 1-3, normalized by the addition of a constant so that $u(0,0) = 0$. In figure 1 the surface height $u(0,y)$ along the symmetry line is shown for several contact angles γ. The behavior of the solution along other mesh lines in the "y direction" differs very little from that along $u(0,y)$.

In figure 2, the variation of the surface height with x is depicted for several values of y for the case $\gamma = 58^\circ$. Note that the optimal curve Γ_0, along which the solution surface would become vertical for the critical contact angle 57.6°, is a circular arc of radius 1.444 intersecting the symmetry line $x = 0$ of the trapezoid at $y = 17.6$ and the slant edge at $y = 17.4$.

In figure 3 are depicted the surface heights $u(0,y)$ for a sequence of trapezoids ranging from the rectangle ($a = 2$) to the almost-critical one ($a = 1.3$), for $\gamma = 58^\circ$. The tendency toward verticality is noticeable as criticality is approached.

4. On the gradient of the solution

Figure 1 indicates that for γ close to the critical angle the graphs have inflection points where the derivative u_y is maximal. The maximum of u_y appears to occur in a small neighborhood of the curve Γ_0 for which the minimum in the estimate (6) is realized. This property is not incidental. Actually Γ_0 is the curve along which a discontinuity of the solution may arise. Namely, $\frac{\partial u}{\partial n}|_{\Gamma_0} \to \infty$ as $\gamma \to \gamma_0$, where $\frac{\partial}{\partial n}$ is differentiation with respect to the outward normal to Γ_0. More precisely, the following is valid.

Theorem: Let a solution to the problem (1) and (2) exist for $\gamma > \gamma_0$, where γ_0 is defined by the equality

$$\cos \gamma_0 = \min_{\Gamma} \frac{\Omega\Gamma}{|\Sigma^* \Omega - \Omega^* \Sigma|} \tag{6a}$$

and let Γ_0 realize the minimum in (6a). Then

$$\left| \int_{\Gamma_0} \frac{1}{W} \nabla u \cdot n \, ds \right| \to \Gamma_0 \tag{7}$$

as $\gamma \to \gamma_0$.

Proof: Let $\delta > 0$ be small and

$$\cos \gamma_0 > \cos \gamma > \cos \gamma_0 - \delta \ .$$

Applying the divergence theorem to the domain Ω^* defined by Γ_0, we have

$$\Sigma^* \cos \gamma + \int_{\Gamma_0} \frac{1}{W} \nabla u \cdot n \, ds = \Omega^* \frac{\Sigma \cos \gamma}{\Omega} \tag{8}$$

Let $\Omega^* \Sigma - \Sigma^* \Omega > 0$ (otherwise we can obtain the necessary estimate for $-\int_{\Gamma_0} \frac{1}{W} \nabla u \cdot n ds$), then it follows

$$\int_{\Gamma_0} \frac{1}{W} \nabla \cdot n \, ds = (\Omega^* \Sigma / \Omega - \Sigma^*) \cos \gamma > (\Omega^* \frac{\Sigma}{\Omega} - \Sigma^*) (\frac{\Gamma_0 \Omega}{\Sigma \Omega^* - \Sigma^* \Omega} - \delta)$$

$$= \Gamma_0 - \delta (\Omega^* \frac{\Sigma}{\Omega} - \Sigma^*) \rightarrow \Gamma_0$$

as $\delta \rightarrow 0$.

The theorem is in a sense an inverse to Concus and Finn's estimate of the critical angle (6).

By usual means it can be derived from the theorem (by assumption of the regularity of the solution) the property that $\partial u / \partial n$ goes to infinity on Γ_0, as $\gamma \rightarrow \gamma_0$.

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Figure Captions

Figure 1. $u(0,y)$ vs. y for contact angles 75^{o}, 60^{o}, 59^{o}

Figure 2. $u(x,y_i)$ vs. x for $y_i = 0,9,15,17.5,20,25$; $\gamma = 58^{o}$

Figure 3. $u(0,y)$ vs. y for $a = 2,1.5,1.4,1.3$; $\gamma = 58^{o}$

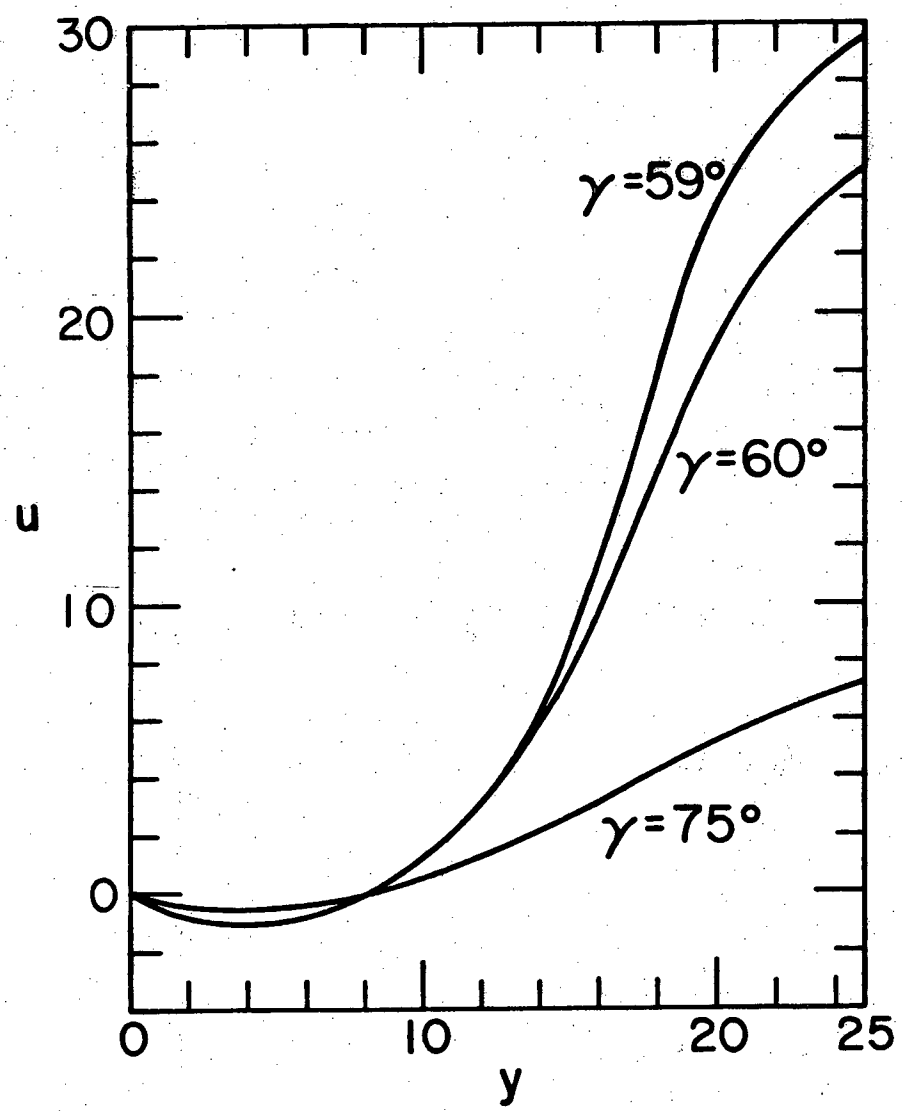

Figure 1

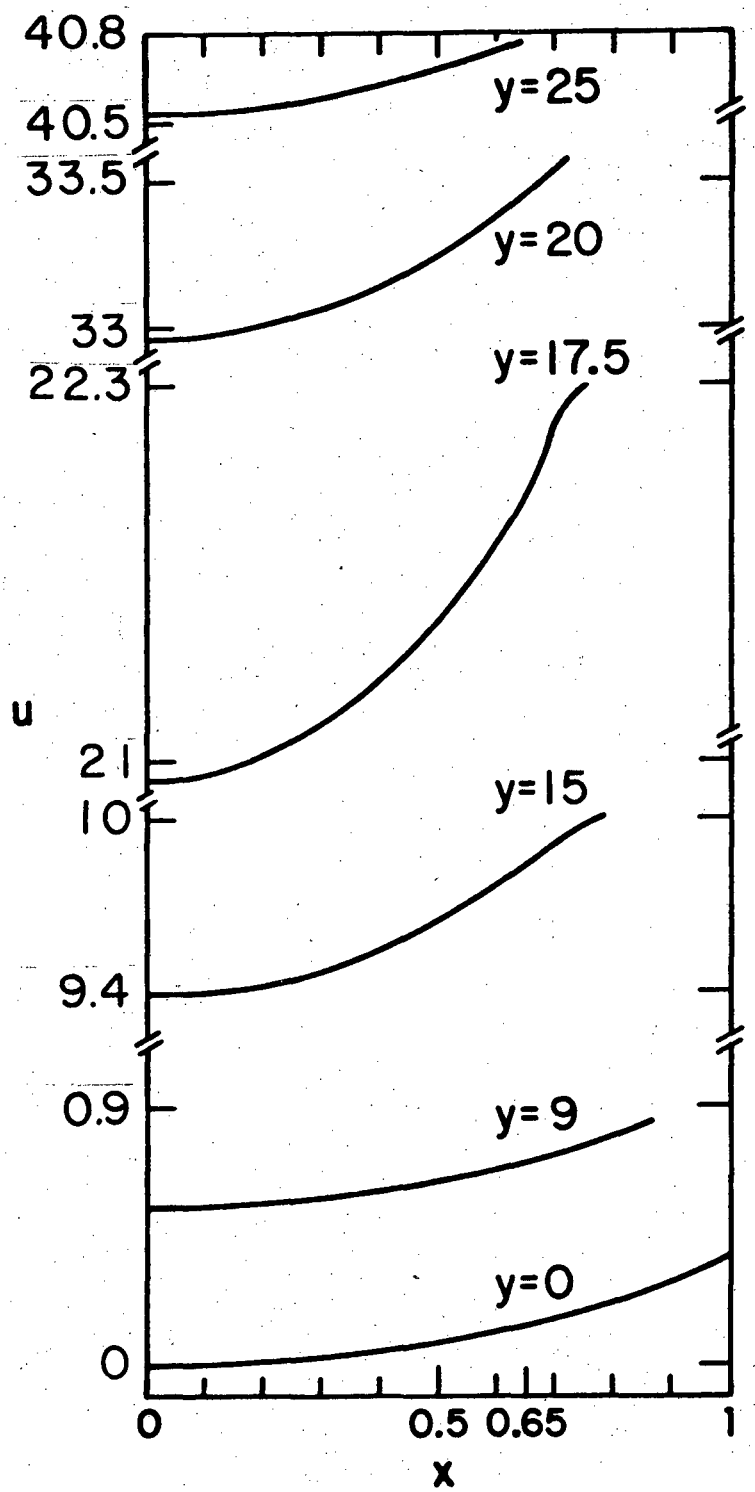

Figure 2

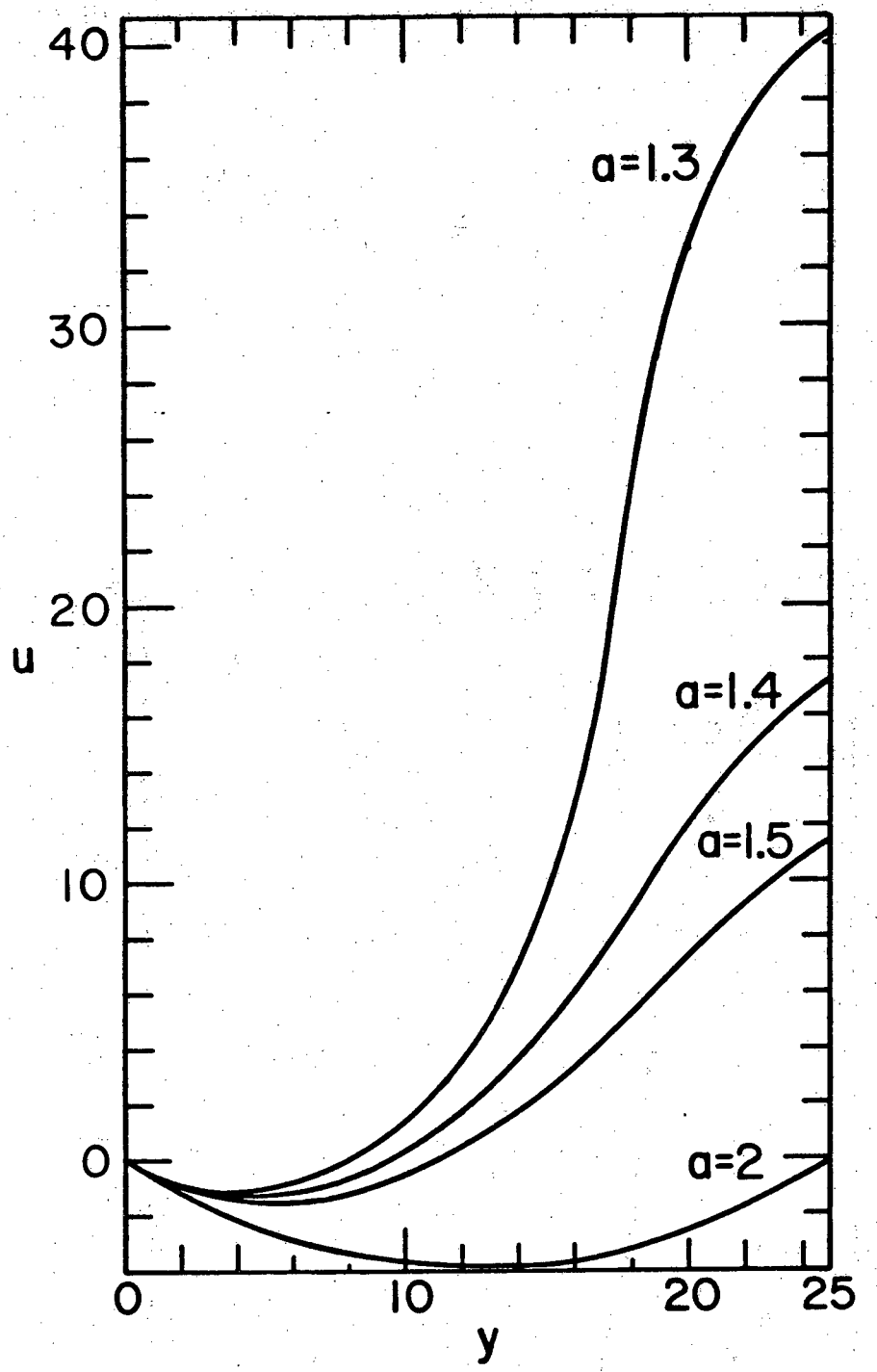

Figure 3

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