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EQUILIBRIUM LIQUID FREE-SURFACE CONFIGURATIONS: MATHEMATICAL THEORY AND SPACE EXPERIMENTS

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Abstract

Small changes in container shape or in contact angle can give rise to large shifts of liquid in a microgravity environment. We describe some of our mathematical results that predict such behavior and that form the basis for physical experiments in space. The results include cases of discontinuous dependence on data and symmetry-breaking type of behavior.

Introduction

In reduced gravity, fluids can behave in striking ways that are different from what occurs in common experience in a terrestrial environment. Discussed here are some of the results underlying such behavior that arise out of our mathematical studies, along with observations from earlier physical experiments in microgravity environments. The results are described in connection with two planned experimental investigations, designed jointly with Mark Weislogel of NASA Lewis Research Center, that are scheduled to be carried out in the glovebox facility on space station *Mir* this year.

Formulation

Our mathematical work is based on the classical Young-Laplace-Gauss formulation for an equilibrium free surface of liquid partly filling a container or otherwise in contact with solid support surfaces. In this formulation, when gravity is absent or can be neglected, which is the situation we discuss here, the mechanical energy E of the system is given by

$$E = \sigma(S - S^* \cos\gamma). \qquad (1)$$

The interfacial liquid-vapor surface tension parameter σ and the relative adhesion coefficient $\cos\gamma$ of the liquid with the container walls are assumed to depend only on the material properties, which are taken here to be homogeneous (the same value of $\cos\gamma$ on all parts of the container, as is the case for the experiments). S and S^* are, respectively, the areas of the liquid-vapor free surface and of the solid-liquid interface.

Equilibrium configurations are those providing stationary values of the energy functional E subject to the condition of fixed liquid volume.[1] The equilibrium liquid-vapor free surfaces so determined are surfaces of constant mean curvature meeting the bounding walls with contact angle γ. We consider here values of the contact angle $0 < \gamma < \pi$. Of particular interest in our mathematical studies are situations in which small changes in contact angle or geometry can result in large changes, possibly discontinuous, of the equilibrium fluid configuration.

The wedge – discontinuous behavior

The first example of discontinuous behavior that we uncovered arose in our study of the problem of a free surface in a wedge (Fig. 1).[2] Consider a cylindrical container, with cross section Ω, closed at one end and partly filled with liquid forming a free surface $\mathcal{S}$. Suppose the cross-section boundary has an isolated corner P of opening angle 2α, $0 < 2\alpha < \pi$, forming a local "wedge domain" at P. One seeks a free surface $\mathcal{S}$, as shown in Fig. 1, that is (locally) represented by a single-valued function over some neighborhood of P in Ω, and which meets the walls that abut at P in a prescribed angle γ. Our results state that *for such a surface to exist the condition* $\left|\gamma - \frac{\pi}{2}\right| \le \alpha$ *must hold.*[1,2,3]

Discontinuous change in behavior at $\left|\gamma - \frac{\pi}{2}\right| = \alpha$ can be illustrated directly for the container in Fig. 2, for which the boundary of the section Ω is completed by joining smoothly to a wedge a circular arc with center on the angle bisector. Over the entire range $\left|\gamma - \frac{\pi}{2}\right| \le \alpha$ an explicit closed-form solution can be given for $\mathcal{S}$, which, for sufficient specified liquid volume, covers the base entirely. It is a portion of a hemispherical surface that meets

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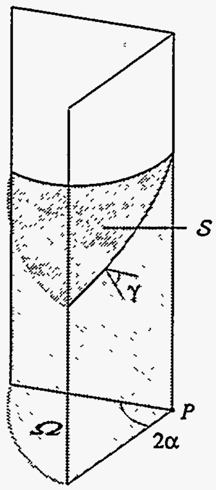

Figure 1. Wedge configuration.

the walls with angle γ. Thus the free surface height is bounded uniformly at P over this range. However, for $|\gamma - \frac{\pi}{2}| > \alpha$ such a surface cannot exist, and the liquid will necessarily move to the corner and uncover the base, rising arbitrarily high at the vertex if $\gamma < \frac{\pi}{2}$ (or falling arbitrarily low if $\gamma > \frac{\pi}{2}$), regardless of liquid volume. *The surface behavior changes discontinuously when* $|\gamma - \frac{\pi}{2}| - \alpha$ *crosses the value zero.*

The discontinuous change in behavior has been corroborated for certain cases in microgravity experiments[1,4,5] and will be investigated in one of the vessels making up our second experiment. The vessel is similar to that in Fig. 2 except that Ω is altered somewhat, to permit the vertex angle 2α to be varied during the experiment. This will allow the cases of advancing and receding liquid motion to be studied. Discontinuous behavior in the wedge also enters into other parts of the second experiment, which are discussed in detail in that section

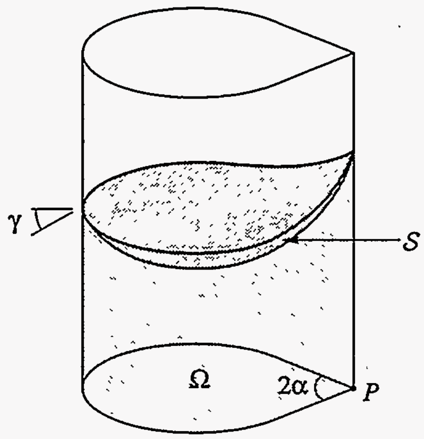

Figure 2. Wedge container.

below. First we turn to a different phenomenon, the one forming the basis of our first experiment on *Mir*.

First experiment

The first experiment, scheduled for the current *Mir* 21/NASA 2 Mission, concerns the behavior of liquid in "exotic" containers. These containers, which are rotationally symmetric, have the remarkable property that for given contact angle and liquid volume, there is an infinity (in fact, an entire continuum) of distinct rotationally symmetric equilibrium configurations, all of which have the same energy.[6,7] The special case of contact angle $\pi/2$ and zero gravity is studied in Ref. 6, where the authors derive a closed form solution; the general case is studied in Refs. 7 and 8.

Fig. 3 depicts the axial section of an exotic container (for the case $\gamma = 80°$ and zero gravity). The toroidal-like bulge of such a container is given by the solution of a nested set of ordinary differential equations.[7,8] This bulge forms the "exotic" portion; it is joined to circular cylindrical extensions with disk ends for the container shown in Fig. 3. The dashed curves in Fig. 3 depict members of the continuum of rotationally symmetric equilibrium interfaces having the same contact angle and energy and enclosing the same volume of liquid with the base. Such containers can be constructed for any contact angle. They can be constructed even for non-zero gravity, but only under microgravity con-

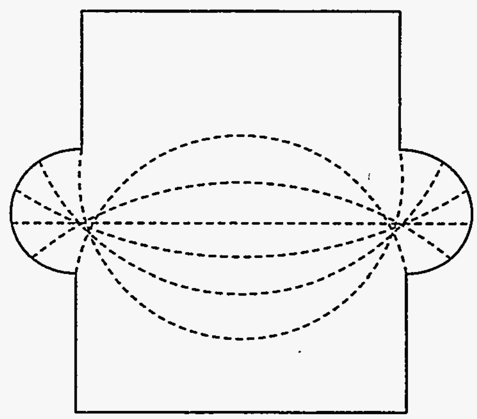

Figure 3. Axial section of an exotic container for contact angle 80° and zero gravity, depicting meridians (dashed curves) of members of the rotationally-symmetric equilibrium free surface continuum. All surfaces have the same contact angle and energy and enclose the same volume of liquid with the bottom of the container.

ditions are they of sufficiently large scale to permit accurate physical experiment and observation.

All of the rotationally-symmetric equilibrium configurations turn out to be unstable, and it can be shown that particular deformations that are not rotationally symmetric yield configurations with lower energy.[7,9] For the container in Fig. 3, for which the ends are sufficiently far apart to exclude a stable columnar liquid bridge between them, it is possible to demonstrate that *any interface that minimizes energy cannot be rotationally symmetric.* This is in notable contrast with what happens in the familiar case of the right circular cylinder, for which the symmetric interface is stable, and no asymmetric ones can appear.[10]

Numerical computations, which make use of the Surface Evolver software package,[11] were carried out to indicate what stable configurations there might be.[12,13] The Surface Evolver seeks local minima of a discretized energy functional, such as (1), subject to prescribed constraints, by employing gradient-descent type methods. Surfaces are approximated by a piecewise-linear triangulation, the form of which can be controlled to various degrees with commands available to the user. Under control of the user, the program adjusts the triangulated surface, step-by-step, in an attempt to decrease the energy. From the numerical and graphical output provided by the program, a user interprets whether a local minimum has been found.

Computed interfaces for the case $\gamma = 80°$ and zero gravity are shown in Figs. 4 and 5. The upper configuration is the local minimum with lowest energy found numerically. The lower figure shows a calculated apparent local minimum configuration with larger energy, but still less than that for the rotationally symmetric continuum. The value $\gamma = 80°$ corresponds to materials used in preliminary drop tower experiments[14] and to one set of materials used in our Interface Configuration Experiment (ICE), joint with M. Weislogel, that was carried out in the glovebox on the NASA USML-1 Space Shuttle Mission. In these experiments a configuration very much like the one shown in Fig. 4 was observed. In the space experiment, where there was opportunity to investigate stability, the configuration was found to be stable even to large disturbances. In the present *Mir* 21/NASA 2 experiment an attempt is made to obtain other equilibria, like the numerically computed one in Fig. 5, and to examine their stability.

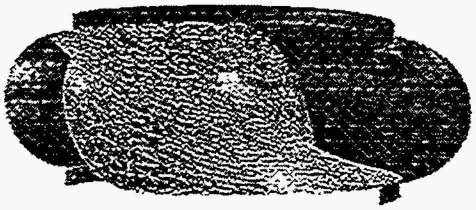

Figure 4. View of calculated energy-minimizing equilibrium interface in an exotic container. Zero gravity, $\gamma = 80°$.

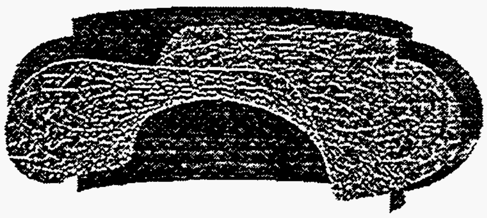

Figure 5. View of calculated larger-energy equilibrium interface in an exotic container. Zero gravity, $\gamma = 80°$.

<u>Second experiment</u>

The second experiment, the Angular Liquid Bridge investigation scheduled for the *Mir* 23/ NASA 4 Mission, is designed to explore more general liquid configurations in a wedge than the one shown in Fig. 1. Impetus for this experiment arises largely from recent doctoral dissertations of two students associated with our study, John McCuan[15] and Lianmin Zhou,[16] from whose contrasting results striking inferences can be drawn.

<u>Liquid bridge in a wedge</u>

In his work, McCuan found conditions under which an equilibrium tubular bridge in a wedge domain (Fig. 6) would be possible in zero gravity, and he gave the shape such a bridge might take. As before, consider a wedge domain with opening angle 2α, $0 < 2\alpha < \pi$. The results McCuan proved contain the following (if the contact angles on the two sides of the wedge are different, the results hold if γ on the left of the inequalities is their average):

If $\gamma > \pi/2+\alpha$, *a bridge in the shape of a portion of a sphere making contact angle* γ *with the walls exists.*

If $\gamma \leq \pi/2 + \alpha$, *no physically realizable bridge is possible.*

Note that these results complement, in respects, the earlier ones given for the wedge. It has not yet been proved whether or not other shape bridges may

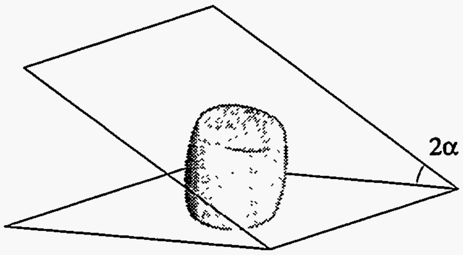

Figure 6. Liquid bridge in a wedge.

be possible when $\gamma > \pi/2 + \alpha$, or whether the spherical bridges are stable (provide a local minimum for the energy). However, our numerical results and those of H. Mittelmann (private communication), obtained using the Surface Evolver software package, indicate that the spherical bridges are stable, at least for the representative cases we considered. Also, no bridge shapes other than the sphere have been found numerically. Note that McCuan's results imply that a bridge is possible only for $\gamma > \pi/2$. A spherical liquid bridge is shown in Fig. 9 for the case $\alpha = 25°$, $\gamma = 130°$.

Bridge between parallel plates – discontinuous behavior

The above results for liquid bridges in a wedge compare in a remarkable way with those for bridges between parallel plates (Fig. 7). This latter problem was studied initially from a rigorous mathematical point of view by Athanassenas[17] and by Vogel[18], and later using a more physical approach by Langbein.[19] (Note that in these papers, as is the case in Ref. 16 and here, the boundary conditions at the plates are prescribed contact angle, which arises from the variational condition for (1). For fixed end conditions, as considered in much of the materials science literature, the behavior of solutions is different.) In her doctoral dissertation, Zhou obtained definitive mathematical results that imply the following:

For any value of the contact angle γ and for any liquid volume V greater than or equal to a critical value $V_0(\gamma)$, a unique stable liquid bridge exists between two parallel plates of given separation.

It is known that any equilibrium bridge must be rotationally symmetric,[18,20] and that its free surface is a Delaunay surface.[16,21,3] For $\gamma > \pi/2$ and for a specific liquid volume $V_s(h)$ depending on the plate spacing h, the free surface is simply a portion of the surface of a sphere. For other values of the volume the Delaunay surface is different from a sphere.

These results, when combined with the results for the wedge, imply that a bridge between parallel plates may change its configuration and position markedly when one of the plates is tilted, even by a small amount, or it even may cease to exist as a bridge altogether; *a liquid bridge between parallel plates can behave discontinuously with respect to tilting of the plates.* In stability studies such as in Refs. 16, 18, and 19, limited to the parallel plate geometry, this liquid bridge instability with respect to plate tilt is not observed.

As a specific example to illustrate the possibilities, consider the case $\gamma > \pi/2$ and a bridge with volume V_s between parallel plates of spacing h, so that the bridge is spherical. Suppose the top plate is tilted clockwise by an angle $2\alpha < 2\gamma - \pi$ about a pivot line in the plate that is a distance $\frac{1}{2}h\tan\alpha$ from the symmetry axis of the bridge. Then this particular bridge remains an equilibrium one for the new tilted plate configuration, without any change in the radius of the sphere or in the bridge's position on the lower plate. However, a bridge with any volume V different from V_s (and with the same contact angle) would change both position and shape discontinuously in altering to a spherical bridge in conjunction with the tilt, shifting to the right for $V < V_s$ or to the left for $V > V_s$.

For $\gamma \leq \pi/2$ an initial bridge would always behave discontinuously with respect to the tilt, regardless of volume, as it cannot persist as a bridge. It has to be expected that the liquid will jump to the edge of the plates in this case. If the tilted plates touch forming a wedge, then configurations described in the following section may form. The above phenomena are ones we wish to study in our forthcoming experiment.

Other configurations

When the conditions for a bridge in a wedge

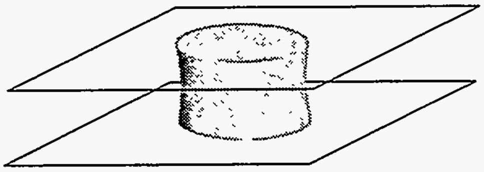

Figure 7. Bridge between parallel plates.

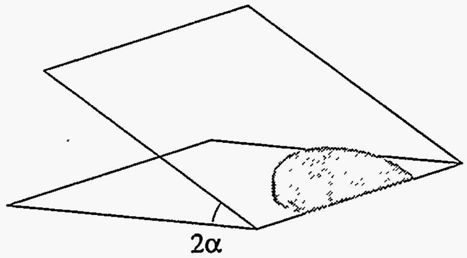

Figure 8. Edge blob in a wedge.

are not satisfied, liquid may assume a position as a blob in the shape of a portion of a sphere in contact with the edge, see Fig. 8. The condition for such a configuration to be possible is that $|\gamma - \pi/2| \leq \alpha$. (Recall we consider here only the case $0 < 2\alpha < \pi$.) Although the edge blobs have not been studied with the same mathematical completeness as have the bridges, they have been noted in Refs. 22 and 23 and for some examples studied numerically. Our numerical computations indicate that, as for the angular bridges, the spherical edge blobs are stable, and as yet we have found no other edge blob shapes numerically.

In our earlier work, discussed above, we have shown that if $\alpha + \gamma < \pi/2$, then fluid cannot remain as a blob in the edge but must spread arbitrarily far along the edge. See also Ref. 23 and the references there for a discussion of stability of liquid columns in a wedge.

Anticipated experiment behavior

The liquid behavior one might expect in a physical experiment in space, based on the Laplace-Young-Gauss formulation, is summarized in Fig. 9. This figure illustrates the information discussed above, based in part on mathematically rigorous results and, where these are not available, on computational evidence for particular cases. The numerical solutions depicted in Fig. 9 were obtained using the Surface Evolver software package. The computations were carried out with initial approximations and transitions between configurations similar to those in which the experiment is designed to proceed, thereby enhancing appropriateness of the numerically based predictions on uniqueness and stability.

The upper two rows of Fig. 9 depict the nonwetting case $\gamma > \pi/2$: A liquid bridge between parallel plates is convex (part of a sphere for a specific fluid volume). Spherical tubular bridges and edge blobs exist for tilted plates, for the range of values indicated. Edge spread is not possible. For fixed $\gamma > \pi/2$, transition from tubular bridges to edge blobs occurs as α increases through the value $\gamma - \pi/2$.

For the wetting case $\gamma < \pi/2$, a liquid bridge between parallel plates is concave. A tubular bridge between tilted plates is not possible, but the (spherical) edge blob and edge spread are. For fixed $\gamma < \pi/2$, the transition from edge blob to unbounded edge spread occurs as α decreases through the value $\pi/2 - \gamma$. Computed edge blobs are shown (from different viewing perspectives) for the case $\alpha = 25°$, $\gamma = 100°$ in the second row and for $\alpha = 20°$, $\gamma = 75°$ in the bottom row.

The planned experiment will explore the transition between the configurations for a nonwetting and for a wetting fluid. As discussed above, when initially parallel plates are tilted, the fluid is predicted to behave discontinuously in general, the exception being the special case of a spherical bridge and a particular pivot line. The other transitions, horizontally across the second and fourth rows of Fig. 9 as α changes value, are gradual, as can be demonstrated by the explicit spherical solutions.

Concluding remarks

We have described fluid behavior predicted mathematically and computationally for the current investigation on the *Mir* 21/NASA 2 Mission and the forthcoming investigation on the *Mir* 23/NASA 4 Mission. The predictions, which include discontinuous behavior, are based on the idealized classical Young-Laplace-Gauss formulation. In the experiments there will be an opportunity to check the predictions against physical behavior and to observe the effects of hysteresis and other phenomena not included in the classical formulation.

Acknowledgments

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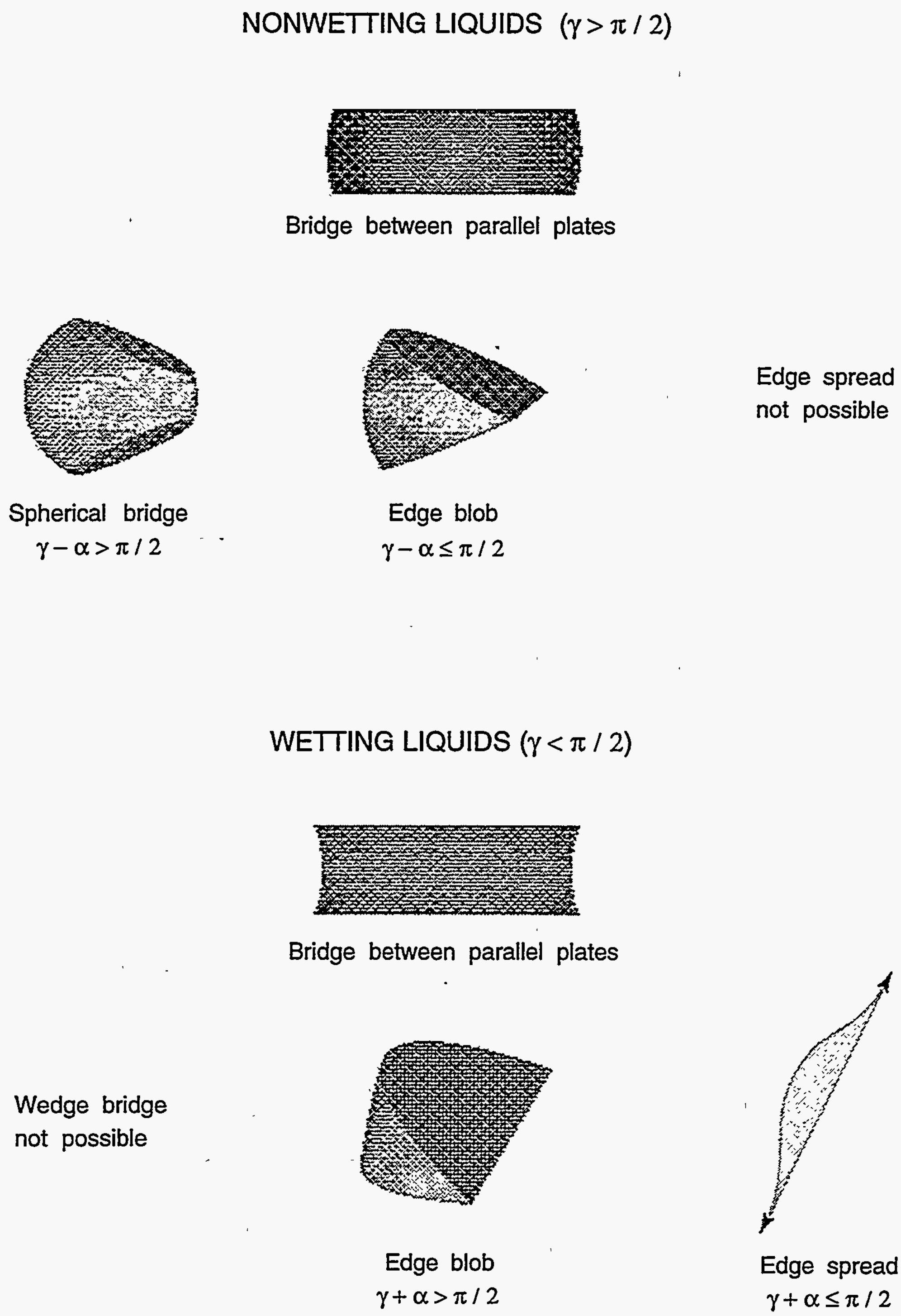

Figure 9. Fluid configurations for second experiment. Upper two rows: nonwetting liquids; lower two rows: wetting liquids.

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