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# Symmetric Capillary Surfaces in a Cube

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# SYMMETRIC CAPILLARY SURFACES IN A CUBE[1]

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# Symmetric Capillary Surfaces in a Cube

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**Abstract**

Numerical experiments are described by which stable capillary surfaces are calculated. The surfaces in question are determined by the following data: the container is a cube in space; the contact angle is $70^0$; the Bond number is zero; only symmetric configurations are taken into consideration.

## 1 The Mathematical Problem

Let $\Phi$ be the unit cube in $\mathbf{R}^3$. We are considering subdomains $\Omega \subset \Phi$ having a piecewise smooth boundary $\partial\Omega = \Gamma \cup \Sigma$, where $\Gamma$ is a subset of the interior of $\Phi$ and $\Sigma$ is a subset of the boundary $\partial\Phi$ of $\Phi$. We are looking for those subdomains $\Omega$ which solve the following variational problem: The energy functional

$$E = \int_\Gamma d\Gamma - \cos\vartheta \int_\Sigma d\Sigma$$

is minimal under the restriction that the volume

$$V = \int_\Omega d\Omega$$

attaines a prescribed value. It is a well known fact - going back to K. F. Gauß - that solutions of this variational problem must be such that the *capillary surface* $\Gamma$ has constant mean curvature

$$2H = p$$

and the *contact angle* between $\Gamma$ and $\Sigma$ equals to $\vartheta$ (see, e.g., [6]). The number $p$ is the Lagrange multiplier of the variational problem. It turns out that it is equal to the difference of the pressures of two liquids (fluid or gas) occupying the domains $\Omega$ and $\Phi \setminus \Omega$, resp.

So far, for the problem studied here, namely capillary surfaces in a cube under zero gravity conditions, there are no existence nor uniqueness proofs, except for simple cases, namely for those in section 3. Nevertheless, the results presented in this paper are consistent with laboratory experiments that have been performed up to now.

There are several papers dealing with similar problems. The problem of determining shapes of capillary surfaces experimentally, mathematically, and numerically for zero gravity conditions has been studied in [5], [8] and [11], see also [15]. In [4] the package EVOLVER was used to determine the shape of equilibrium capillary surfaces for exotic containers. The same package was used for the numerical studies of the present paper, see section 4. A numerical method that allows solving the Euler-Langrange equation for the variational problem described above has been presented in [9]. This method, and also the EVOLVER, allows calculating surfaces that are not simple graphs of functions over a planar domain; i.e., more complicated geometrical configurations can be treated rather than only projectable surfaces. The following is known for a semi-infinite cylindrical tube of general cross section with gravity zero (or positive): If the boundary of the free surface lies entirely on the cylindrical walls, then the surface is determined uniquely by its contact angle and volume, see [13]. Therefore, in that case the standard numerical methods determine a uniquely defined solution, if it exists. In the more general case of a finite container such as a cube, there is no uniqueness result of that type. This lack of uniqueness makes the numerical computations especially important.

A more recent study of bifurcation phenomena for problems with axial symmetry is given in [10]. There, for drops that are entrapped between two parallel planes, numerical methods were used that depend strongly on path-following techniques, see [1] and [14].

## 2 Symmetric Configurations

In this paper we restrict ourselves to domains that share symmetries with the cube. It is obvious that after prescribing the contact angle $\vartheta$ and the volume $V$ and then finding a solution $\Omega$ of the variational problem, the set $\tilde{\Omega} = \Phi \setminus \Omega$ solves the variational problem for the data $\tilde{\vartheta} = \pi - \vartheta$ and $\tilde{V} = 1 - V$. Conversely, if we prescribe $\tilde{\vartheta} = \pi - \vartheta$ and $\tilde{V} = 1 - V$ and find the set $\tilde{\Omega}$, we get a solution of the original problem as $\Omega = \Phi \setminus \tilde{\Omega}$. We call this the *complementary configuration.*

In the following we are going to describe the various topological situations and show plots of figures that were obtained numerically for the contact angle $\vartheta = 70^0$. In those cases where the volume $\Omega$ is the union of several unconnected symmetric sets we will show only one of these sets. In order to indicate the container, we also show the bottom face of the cube.

1. **The Corners:** For this situation we assume that $\Omega$ is the union of eight symmetric sets $\Omega_i$, $i = 1, ..., 8$ which are attached to the eight corners of the cube. This case is denoted by "Ce". If $\tilde{\Omega}$ is this union, the complementary configuration $\Omega$ is denoted by "Ci". Obviously, these solutions make sense only as long as the individual sets $\Omega_i$ do not touch each other. Hence, they are taken into consideration only for a range

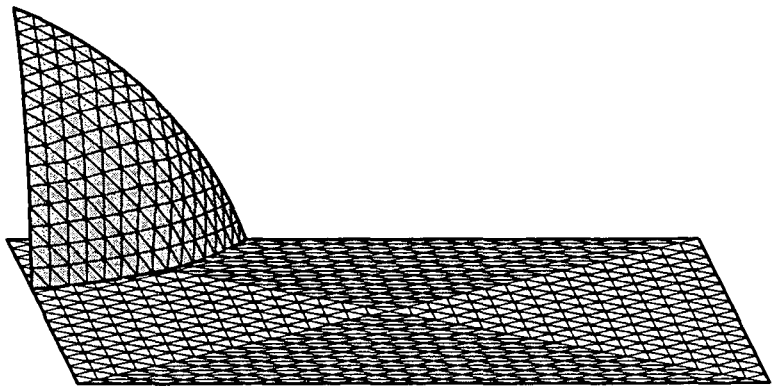

Figure 1: Ce: Exterior Corner, $V = 8 * 0.0125 = 0.1$

of volumes of the form $0 < V < V_{Ce}$ and $V_{Ci} < V < 1$, resp., with some values $V_{Ce}$ and $V_{Ci}$. Figure 1 shows one eighth of $\Omega$ for the case "Ce" with $V = 0.1$.

2. **The Edges:** For this situation we assume that $\Omega$ is the union of four symmetric sets $\Omega_i$, $i = 1, ..., 4$ which are attached to four of the twelve edges of the cube. Each of the $\Omega_i$ is assumed to cover a part of the edge not touching the neighbouring corners. This case is denoted by "Le" (lemon). The complementary situation is denoted by "Li". The domains of existence are $0 < V < V_{Le}$ and $V_{Li} < V < 1$, resp. Figure 2 shows one fourth of $\Omega$ for the case "Le" with $V = 0.08$.

3. **The Faces:** For this situation we assume that $\Omega$ is the union of six symmetric sets $\Omega_i$, $i = 1, ..., 6$ which are attached to the six faces of the cube without touching one of the edges or each other. This case is denoted by "Oe" (orange). The complementary situation is denoted by "Oi". Here we have $0 < V < V_{Oe} = 0.646$ and $0.567 = V_{Oi} < V < 1$, resp., see section 3. Figure 3 shows one sixth of $\Omega$ for the case "Oi" with $V = 0.4$.

4. **Bridges between Two Corners:** For this situation we assume that $\Omega$ is the union of four symmetric sets $\Omega_i$, $i = 1, ..., 4$ which are attached to four of the twelve edges of the cube. Each of the $\Omega_i$ is assumed to cover the whole edge including the neighbouring corners. This case is denoted by "Se" (sausage). The complementary situation is denoted by "Si". Here we have $V_{Se}^- < V < V_{Se}^+$ and $V_{Si}^- < V < V_{Si}^+$, resp. Figure 4 shows one fourth of $\Omega$ for the case "Se" with $V = 0.2$.

5. **Dry Spots:** For this situation we assume that $\Omega$ is the union of two symmetric sets $\Omega_i$, $i = 1, 2$ which are attached to two of the six faces of the cube. Each of

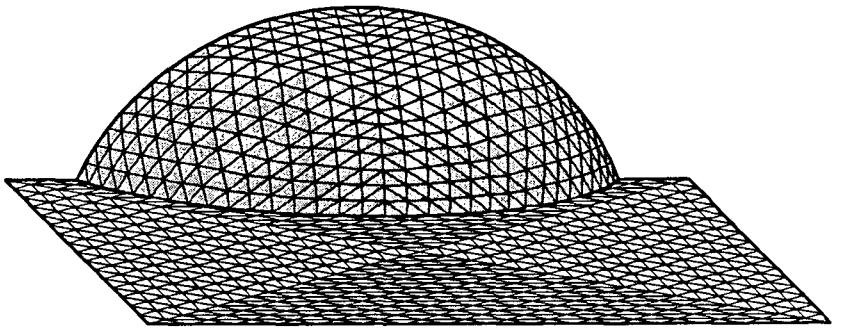

Figure 2: Le: Exterior Lemon, $V = 4 * 0.02 = 0.08$

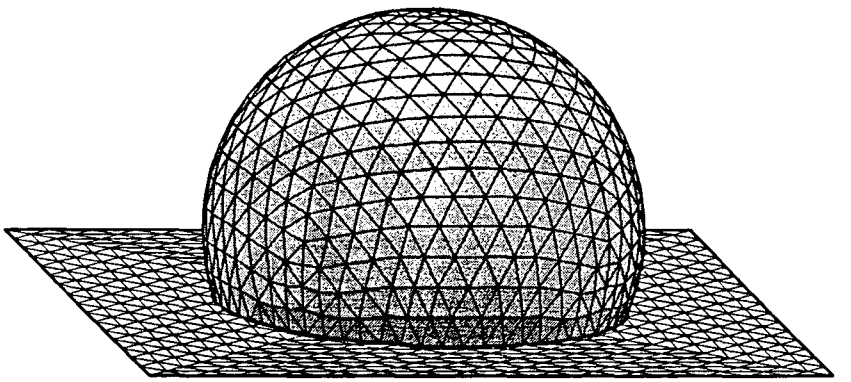

Figure 3: Oi: Interior Orange, $V = 1 - 6 * 0.1 = 0.4$

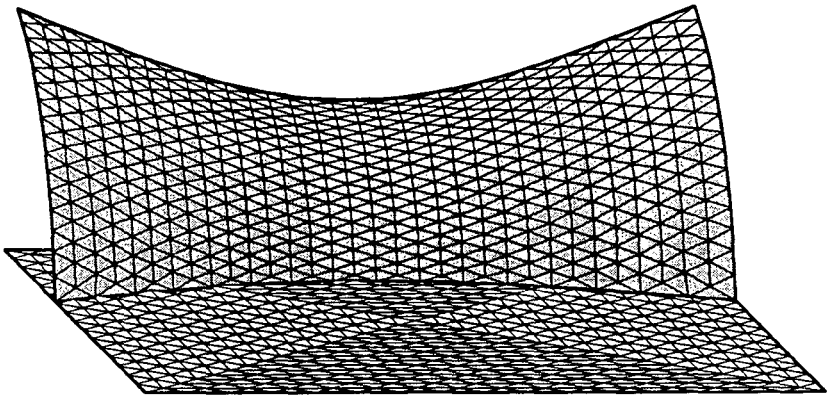

Figure 4: Se: Exterior Sausage, $V = 4 * 0.05 = 0.2$

the $\Omega_i$ is assumed to cover completely the edges that belong to the face including the neighbouring corners but to leave out an uncovered fraction in the interior of the face. This case is denoted by "De". The complementary situation is denoted by "Di". Here we have $V_{De}^- < V < V_{De}^+$ and $V_{Di}^- < V < V_{Di}^+$, resp. Figures 5 and 6 show one half of $\Omega$ for the cases "De" with $V = 0.16$ and "Di" with $V = 0.8$, resp.

6. **The Pumpkin:** For this situation we assume that $\Omega$ is a connected set which covers all eight corners of the cube and also all twelve edges but which leaves out interior parts of all six faces and also a certain volume in the interior of the cube itself. This case is denoted by "Pe". The complementary situation is denoted by "Pi". Here we have $V_{Pe}^- < V < V_{Pe}^+$ and $V_{Pi}^- < V < V_{Pi}^+$, resp. Figures 7, 8, 9, 10, 11, and 12 show the set $\Omega$ for the cases "Pe" with $V = 0.2, 0.5, 0.65$ and "Pi" with $V = 0.2, 0.5, 0.7$, resp.

7. **The Cylinder:** For this situation we assume that $\Omega$ is the union of two symmetric sets $\Omega_i$, $i = 1, 2$ which are attached to two opposite ones of the six faces of the cube covering these faces completely including the neighbouring edges and parts of the neighbouring faces. This case is denoted by "Te" (tub). The complementary situation is denoted by "Ti". Here we have $V_{Te}^- < V < V_{Te}^+$ and $V_{Ti}^- < V < V_{Ti}^+$, resp. Figure 13 shows the set $\Omega$ for the case "Te" with $V = 0.6$.

8. **The Ball:** Here we assume that $\Omega$ is the exterior of a ball that has no contact to any of the six faces of the cube. This case is denoted by "Be". Here we have $V_{Be} < V < 1$.

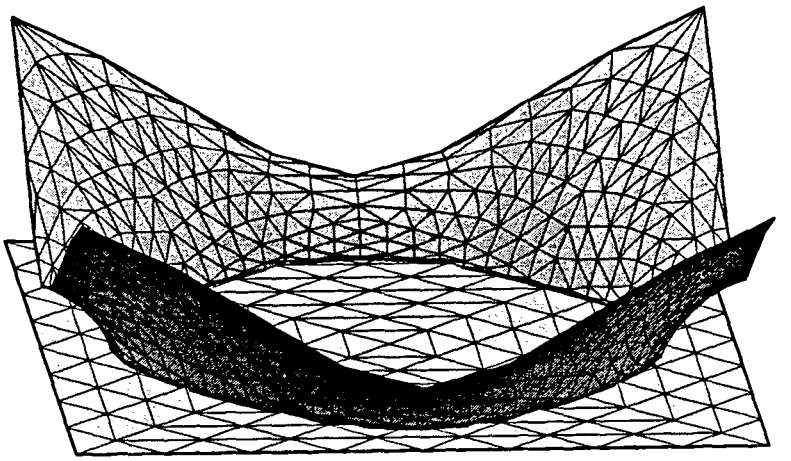

Figure 5: De: Exterior Dry Spot, $V = 2 * 0.08 = 0.16$

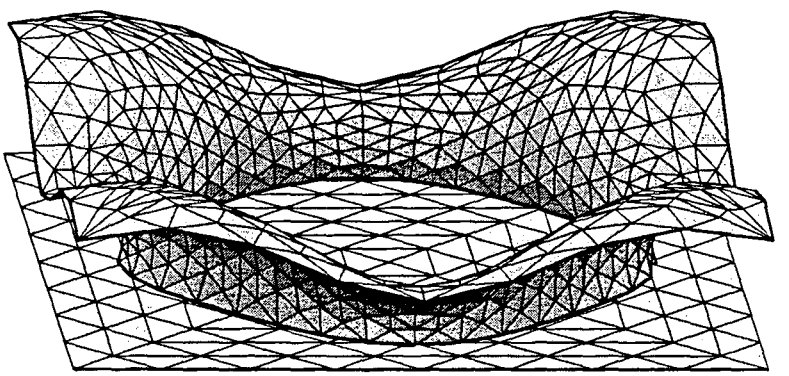

Figure 6: Di: Interior Dry Spot, $V = 1 - 2 * 0.1 = 0.8$

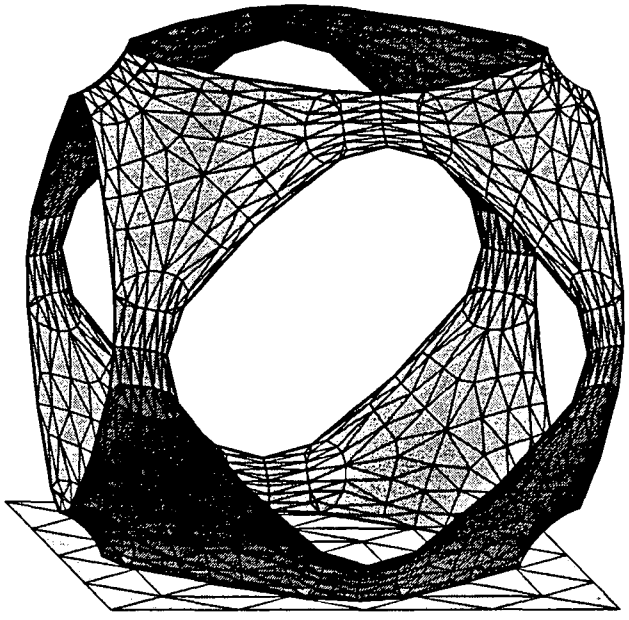

Figure 7: Pe: Exterior Pumpkin, $V = 0.2$

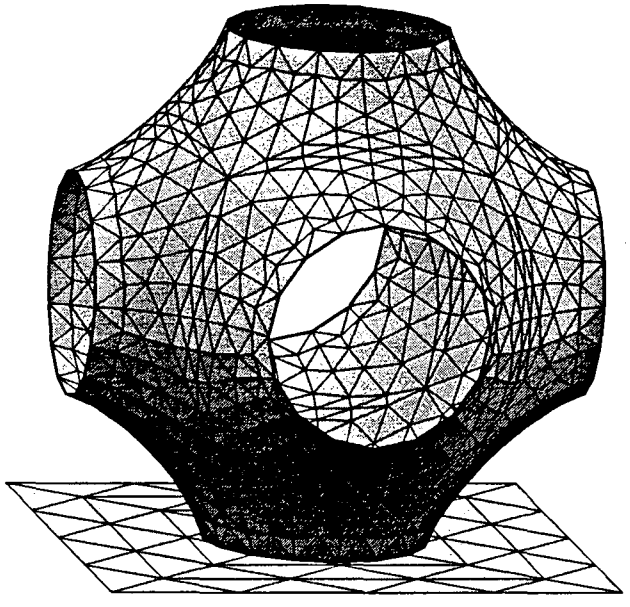

Figure 8: Pe: Exterior Pumpkin, $V = 0.5$

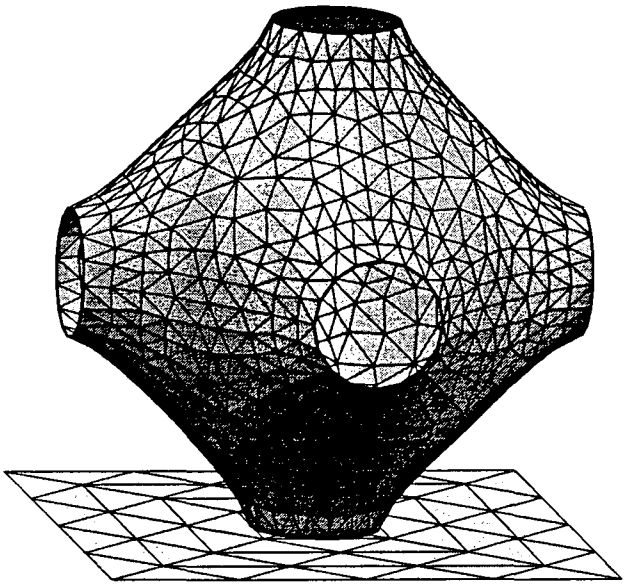

Figure 9: Pe: Exterior Pumpkin, $V = 0.65$

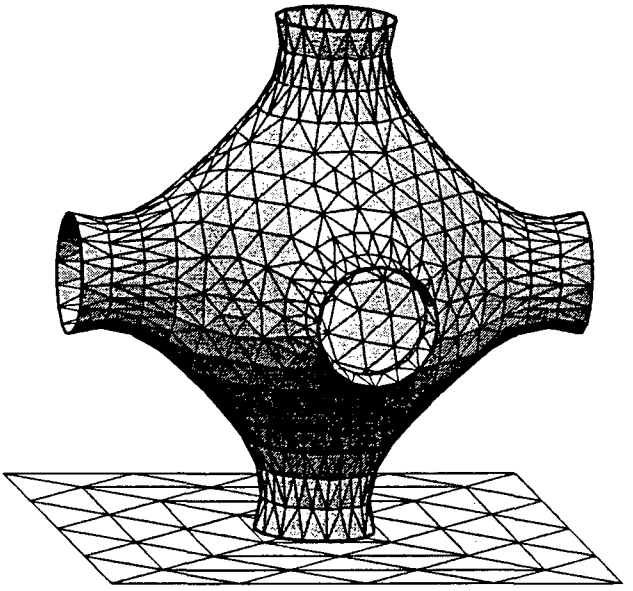

Figure 10: Pi: Interior Pumpkin, $V = 0.2$

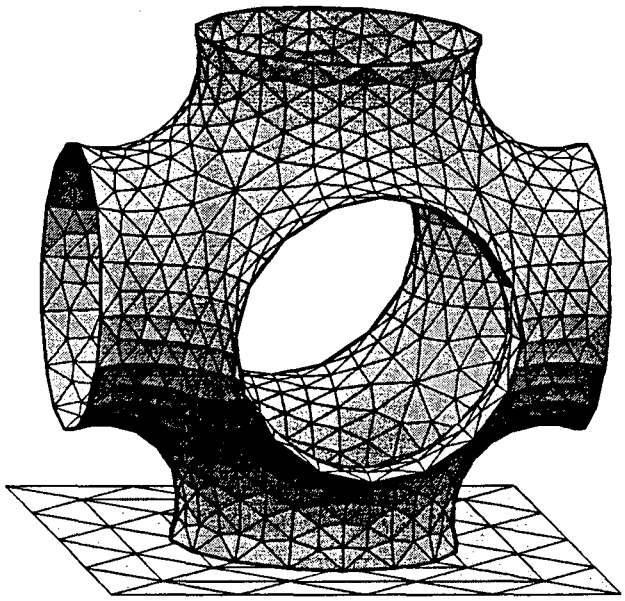

Figure 11: Pi: Interior Pumpkin, $V = 0.5$

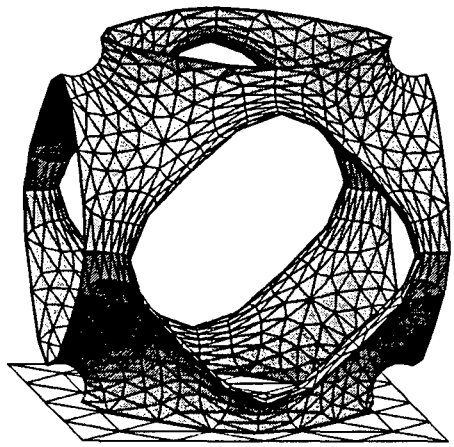

Figure 12: Pi: Interior Pumpkin, $V = 0.7$

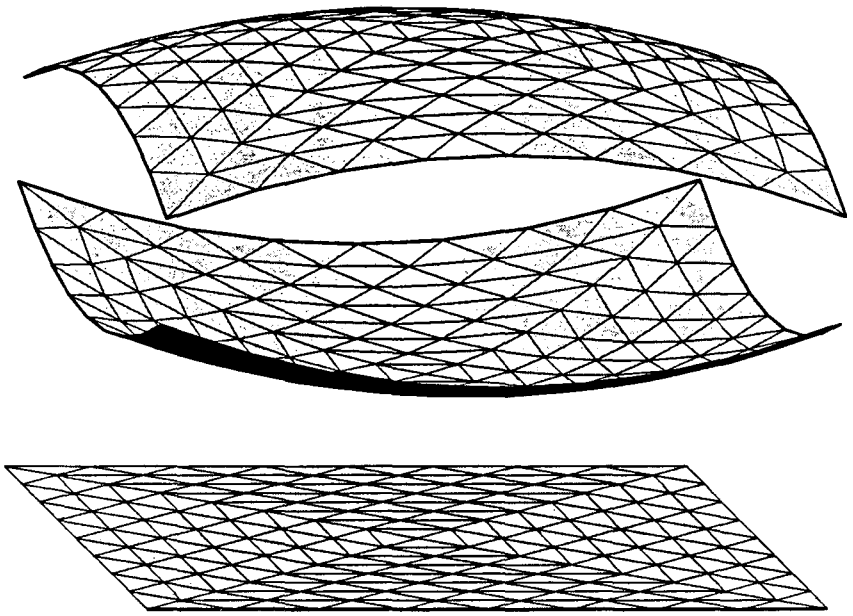

Figure 13: Te: Exterior Tub, $V = 2 * 0.3 = 0.6$

# 3 Results in Closed Form

For simple geometric configurations one can give the volume $V$, the energy $E$, the pressure $p$, and the area $A = \int_\Gamma d\Gamma$ in closed form, see also [7] for formulas in the cases of drops entrapped between two planes.

- **The Ball:** If the domain $\Omega$ is the complement with respect to the cube $\Phi$ of a ball having radius $r$, i.e., in situation "Be", we have the following relations. The volume $V$ and the area $A$ are given by

  $$V = 1 - \frac{4\pi}{3}r^3, \quad A = 4\pi r^2.$$

  Therefore, the energy $E$ is

  $$E = A - \cos\vartheta|\partial\Phi|,$$

  where $|\partial\Phi| = 6$ is the area of the surface of the container. The pressure $p$ is equal to $2H$, where $H = \frac{1}{r}$ is the mean curvature of the surface of the ball, hence

  $$p = \frac{2}{r}.$$

- **The Orange:** If $\Omega$ is one slice of height $h < r$ of a ball which has radius $r$, we have the following relations. With

  $$h = r(1 - \cos\vartheta), \quad s = r\sin\vartheta$$

we have

$$V = \frac{\pi}{3}h^2(3r - h), \quad A = 2\pi r h$$

and

$$p = \frac{2}{r}.$$

Hence, in the situation "Oe" we get for the six slices

$$V_e = 6V, \quad A_e = 6A, \text{ and } E_e = A_e - 6\pi s^2 \cos\vartheta.$$

Simple geometric considerations lead one to the restriction

$$0 < r < r_{max} = \frac{1}{2}\min\{\frac{1}{\sqrt{2} - \cos\vartheta}, \frac{1}{\sin\vartheta}\}.$$

If $\Omega$ is the complement with respect to the ball of a slice cut from the ball, we get the following relations.

$$V = \frac{4\pi}{3}r^3 - \frac{\pi}{3}h^2(3r - h), \quad A = 2\pi r(2r - h)$$

and

$$p = -\frac{2}{r}.$$

Hence, in the situation "Oi" we get for the complement of the six sets of this type

$$V_i = 1 - 6V, \quad A_i = 6A, \text{ and } E_i = A_i - 6(1 - \pi s^2)\cos\vartheta.$$

Here the restrictions to be satisfied are

$$0 < r < r_{max} = \frac{1}{2}\frac{1}{\sqrt{2} + \cos\vartheta}.$$

# 4 Numerical Results

As a test example the case of a contact angle of 70 degrees was chosen. The figures show the results that were obtained by using the program package EVOLVER (see [2] [3]). On the average, for surfaces that have about 1000 vertices one needs 10 steepest descent iteration steps followed by at least 50 conjugate gradient steps to obtain results with sufficient accuracy. Between 500 and 5000 vertices where needed to represent the surfaces. The method underlying this program package is in principle similar to the technique described in [12].

There are curves of the following three relations: Figure 14 shows $E$ versus $V$, figure 15 shows $p$ versus $V$, and figure 16 shows $A$ versus $V$. All these curves are obtained by calculating the solutions using the EVOLVER package. For each of the solutions, one gets not only the surface $\Gamma$ described by its vertices, edges, and faces, but also the values for $V$, $E$, $A$, and $p$. These numerical values were used to draw polygonal lines that connect the points in the $V$-$E$-plane, the $V$-$p$-plane, and the $V$-$A$-plane. Since obviously $p \to \infty$ for $V \to 0$ in the cases "Ce", Le", and "Oe", and $p \to -\infty$ for $V \to 1$ in the cases "Be", "Li", "Ci", and "Oi", the $V$-$p$-curves were cut at $p = 10$ and $p = -10$, resp.

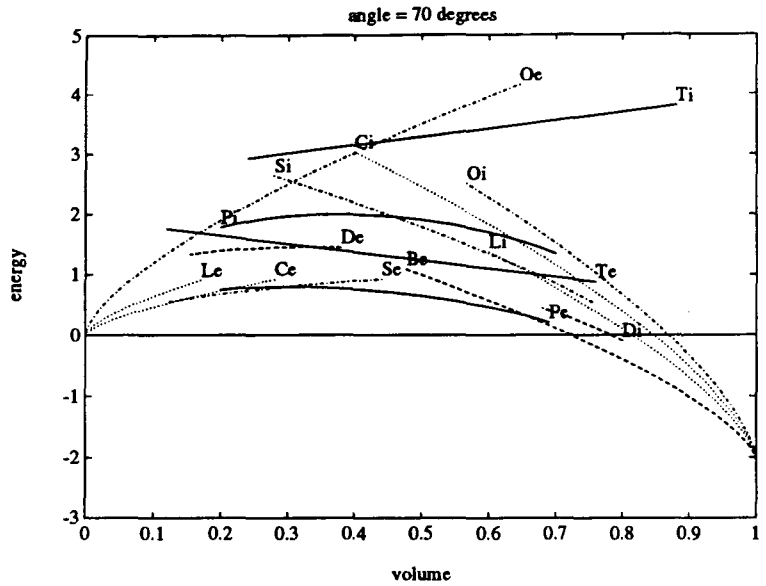


Figure 14: Energy versus Volume

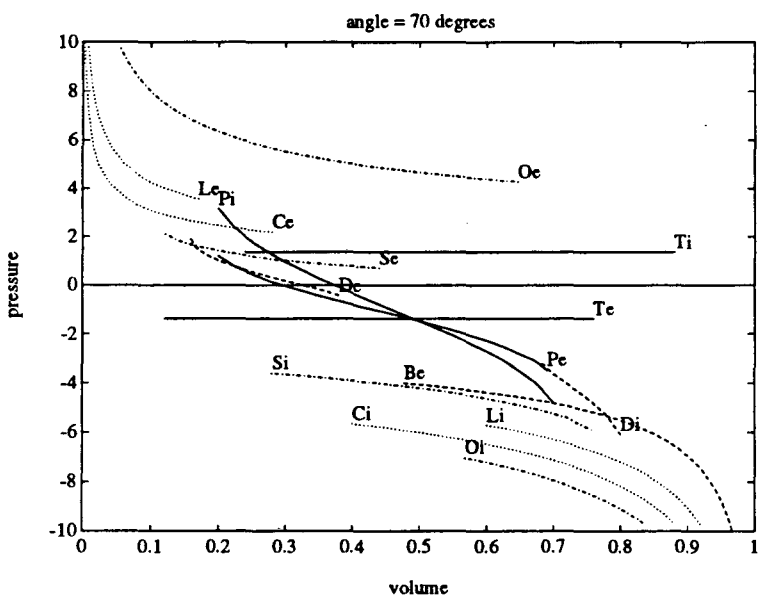


Figure 15: Pressure versus Volume

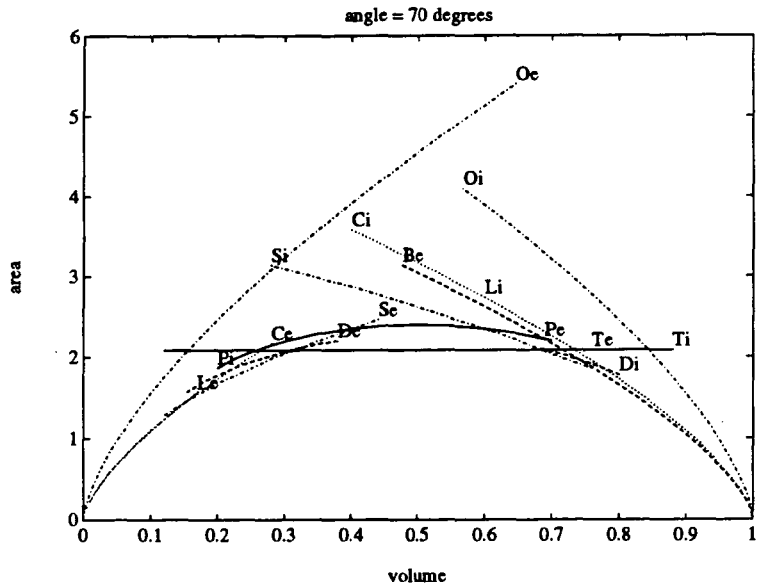


Figure 16: Area versus Volume

## 4.1 Special Properties

If one considers an experiment in which the cube is partially filled with a liquid leaving the complement as void and if one increases the value of the volume $V$ from 0 to 1, the following sequence of stable configurations will result: 1) The corners "Ce", then from $V = 0.145$ on 2) the sausage "Se", after this from $V = 0.301$ on 3) the pumpkin "Pe", and finally from $V = 0.656$ on 4) the ball "Be". This observation is based on the assumption that one considers only configurations with the symmetries described in this paper, and on the other hand, if one looks only for those cases which have the absolute minimum of the energy functional $E$. This means that the other cases for which figure 14 shows larger values of the energy $E$, represent only local minima of the variational problem. In principle, they can be obtained using careful experimental manipulations; but they are only locally stable.

For certain values of the volume $V$ there are quite a few different local minima. As an example, let us look at $V = 0.68$. There are as many as ten different possible configurations for this volume. Here, the values of the energy increase in the following order: "Be", "Pe", "Di", "Li", "Si", "Te", "Ci", "Pi", "Oi", "Ti". It depends on the history of an experiment which of the configurations will actually be observed in a given situation. This is a pronounced *hysteresis* effect.

The curves $p$ versus $V$ are the derivatives $p = \frac{dE}{dV}$ of the curves $E$ versus $V$. This is due to the fact that the Lagrange multiplier of a variational problem is the derivative of the objective function with respect to the value of the constraint. For these curves one can see that for small values of the volume $V$ the pressure $p$ is always positive in this case, whereras it is negative for larger values of the volume. For those cases in which

the pressure happens to be zero, one gets *minimal surfaces* for $\Gamma$, since then the mean curvature $H$ is zero.

The curves $A$ versus $V$ seem to indicate that for the two cases "Pe" and "Pi" one has $A_i(V) = A_e(V)$, i.e., that the areas $A$ are the same for the same volume $V$ prescribed in the two cases.

From the basic concept of the package EVOLVER it is clear that one can get only local minima of the variational problem. It is not possible to calculate other stationary points of the energy functional using this program package. Therefore, the curves in the $V$-$E$-plane leave the branches out which have saddle-points. In this sense, we have calculated only a part of the full bifurcation diagrams. One way of doing that would be to use an approach that has been studied previously in [9].

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