

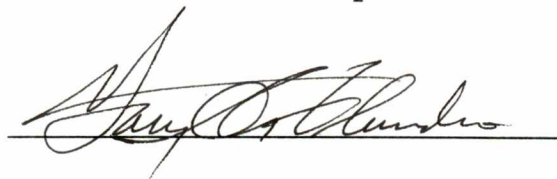
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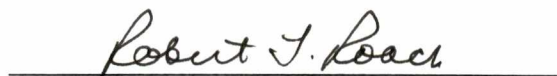
I am submitting herewith a thesis written by Robert Allen Herron entitled "2-D Free Surface Modeling of a Liquid Contained in an Axisymmetric Vessel." I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Engineering Science and Mechanics.



Dr. B. Antar, Major Professor

We have read this thesis and
recommend its acceptance:





Accepted for the Council:



Associate Vice Chancellor
and Dean of the Graduate School

2-D FREE SURFACE MODELING OF A LIQUID CONTAINED IN
AN AXISYMMETRIC VESSEL

A Thesis

Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Robert Allen Herron

December 1995

DEDICATION

This thesis is dedicated to my wife

Sheryl Lynn Herron

whose unconditional love and support was invaluable to me

while completing my degree.

ACKNOWLEDGMENTS

I would like to thank my major professor, Dr. Basil Antar for his guidance in my education and research. I would also like to thank the other committee members, Dr. Gary Flandro and Dr. Robert Roach, for their educational guidance and patience with me. I especially want to express my love and gratefulness to my parents Larry and Kathy Waddell for being there to help and share some of the burdens of life with me , my wife, and son Sean while I was working towards my degree.

ABSTRACT

The emphasis of this research is to determine the free surface shape of a liquid contained in an axisymmetric vessel under the influence of gravitational and centrifugal forces in a microgravity environment. The numerical scheme developed for determining the free surface shape is based on a graphical method developed by Slobozhanin and Tyupstov[7].

The differential equations used in calculating the free surface are the governing equations for the equilibrium free surface line, nondimensionalized in terms of the Bond number and Rotation number, and two equations based on the physical constraints of the problem. The difficulty in the straight forward integration of the equations to obtain the free surface coordinates is due to two unknowns q and r_A . q is an unknown which arises from the development of the governing equations and r_A is the coordinate of the boundary condition satisfied at the vessel wall. The numerical scheme uses a quasi-Newton's method (see [3]) to determine q and r_A to some specified tolerance. After q and r_A are found the

governing equations can be integrated to obtain the coordinates of the free surface line.

The results obtained by the numerical method are in agreement with the results obtained by the graphical method, and in qualitative agreement with results obtained by Concus [4] and the results given in [2].

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CHAPTER 1

INTRODUCTION

With the development and construction of the international space station becoming more feasible, the demand for liquids in space for use in experimental investigations and consumption will increase. Therefore, the management of liquids in a microgravity environment needs to be researched further and maybe in some cases re-examined.

The need for research in the area of microgravity fluid dynamics is to understand the effect of the forces that would act upon a fluid in a microgravity environment. There are forces that would remain the same regardless of the magnitude of the gravitational force, such as surface forces and centrifugal forces. In terrestrial applications, some forces can be neglected because they are much smaller in magnitude compared to the gravitational force. But in a microgravity environment, forces that would normally be neglected in terrestrial applications have to be accounted for since they become comparable to or dominant over the gravitational force. An area of interest is the effect the

microgravity environment has upon the shape of the liquid-vapor interface or the liquid free surface.

The shape of the free surface is dependent upon the forces acting upon the liquid. At the free surface, as the gravitational force decreases, the dominant force becomes the surface tension force. It is the interest of this thesis to determine the shape of the free surface due to rotation as well as the changes in the gravitational and surface tension forces.

The objective is to review an older method developed by Slobozhanin and Tyupstov [8] which determines the free surface shape graphically and to update the method by determining the free surface by a numerical method.

In chapter 2, the governing equations for the axisymmetric equilibrium free surface line are developed. Chapter 3 describes the method developed by Slobozhanin and Tyupstov, and develops the numerical method of determining the free surface. Chapter 4 presents some of the free surfaces calculated by the numerical method and discusses some of the problems encountered in developing the numerical method. Chapter 5 closes with the conclusions about the numerical method and future recommendations.

CHAPTER 2

THE AXISYMMETRIC EQUILIBRIUM FREE SURFACE

The free liquid surface is a condition where a liquid boundary is open to an atmosphere, vapor, or another gas. Free liquid surfaces can be classified into two categories: (1) the classic free surface, where the gas lying over the liquid only imposes a pressure at the liquid-gas interface, or (2) the case where the atmosphere exerts pressure, shear, heat flux, and mass flux at the interface. The free surface investigated in this thesis is the classic free surface shape of a liquid contained in an axisymmetric vessel.

The classic free surface has two required conditions: (1) the fluid particles at the surface must remain at the surface (kinematic condition) and (2) the liquid and the vapor pressures must balance except for surface tension effects. The kinematic condition requires the fluid particle's upward velocity be equal to the motion of the free surface. (see [9])

In this chapter the governing equations for the liquid free surface shape will be developed in accordance with the

classic free surface conditions mentioned above. The boundary conditions will be discussed next, ending with the dimensional analysis of the governing equations.

2.1 DERIVATION OF THE GOVERNING EQUATIONS

The shape of the liquid free surface is determined from the governing equations of the equilibrium free surface line. The governing equations will be developed for axisymmetric vessels where the gravitational force acts along the axis of symmetry. In this case the equilibrium free surface is symmetric with respect to the axis of symmetry of the vessel . To take advantage of the symmetrical nature of the problem , a cylindrical coordinate system (r,θ,z) will be used on a constant θ plane, where the z axis is the axis of symmetry. The coordinate system will also be fixed to the vessel such that if the vessel is rotating the coordinate system will rotate along with the vessel.

Other assumptions maintained in the development of the equations are:

1. the liquid is incompressible and homogeneous

2. the liquid and its vapor, or another gas completely fills the vessel
3. the vessel walls are of a homogenous material and are smooth and rigid
4. there is no motion in the liquid or the vapor adjacent to the liquid
5. adiabatic conditions hold

The body forces considered in the development of the governing equations will only be the gravitational and the centrifugal forces.

The curvature of a free liquid surface can be determined from the application of the second condition of the classic free surface . The second condition is met by applying Laplace's condition for the curvature of the free surface,

$$p_v - p = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right) \quad (2.1.1)$$

where R_1 and R_2 are the principle radii of curvature for the free surface(see Fig. 2.1), p_v is the vapor pressure, and σ is the coefficient of surface tension. Formally stated, the pressure difference between the liquid and

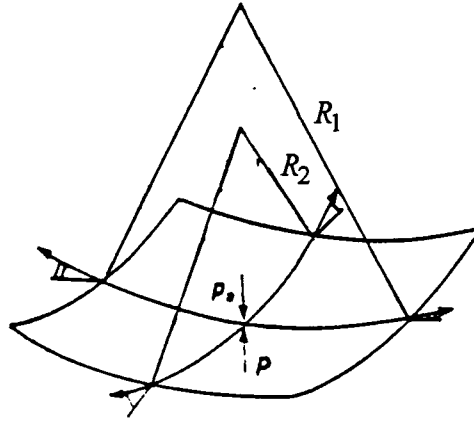


Fig. 2.1: Radii of curvature [8]

the vapor is equal to the surface tension force.

The pressure distribution in the liquid p can be determined from the momentum equations of fluid dynamics

$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + \rho \vec{F}_B + \mu \nabla^2 \vec{v} \quad (2.1.2)$$

where ρ is the liquid density, $\vec{v}$ is the liquid velocity,

$\vec{F}_B$ is the body force, and μ is the liquid viscosity.

Applying the assumption that no motion exists within the liquid or the vapor, the momentum equation can be reduced to the hydrostatic balance:

$$\nabla p = \rho \vec{F}_B \quad (2.1.3)$$

Though rotational velocities are accounted for in the determination of the free surface shape, the assumption that no motion exists within the liquid can be applied because after spinup time has elapsed there is no motion of the liquid relative to the coordinate system.

Since the only body forces under consideration are the gravitational and centrifugal forces, the body force $\vec{F}_B$ will be treated as being derivable from a potential function Π , which will be defined later. Therefore, let

$$\vec{F}_B = -\nabla\Pi \quad (2.1.4)$$

and substitute into eq.(2.1.3). After integrating eq.(2.1.3), the expression for the pressure distribution within the liquid is obtained

$$p = -\rho\Pi + c \quad (2.1.5)$$

where c is a constant of integration. Substituting eq.(2.1.5) for the pressure distribution into eq.(2.1.1), the following equation results

$$\rho\Pi + c = \sigma\left(\frac{1}{R_1} + \frac{1}{R_2}\right) \quad (2.1.6)$$

where p_v has been absorbed into the constant of integration, c .

Next a functional form for the sum of the radii of curvature needs to be determined. For the axisymmetric problem, $R_1 = R_2 = R$ and the sum of the radii of curvature of the surface can be determined from differential geometry and represented parametrically in the form (see [7])

$$\frac{1}{R_1} + \frac{1}{R_2} = \frac{2}{R} = \pm \frac{1}{r \frac{dr}{ds}} \frac{d}{ds} \left(\frac{r \frac{dz}{ds}}{\sqrt{\left(\frac{dr}{ds}\right)^2 + \left(\frac{dz}{ds}\right)^2}} \right) \quad (2.1.7)$$

where the sign is chosen so that the unit normal vector to the surface is directed towards the vapor. s is a parameter that will be taken to be the arc length of the free surface, and r and z are the coordinates of the free surface.

From the geometry of the surface (see Fig. 2.2), the following identities are obtained

$$\sin \beta = \frac{dz}{ds}, \quad \cos \beta = \frac{dr}{ds} \quad (2.1.8a, b)$$

where β is the angle formed by the tangent to the free surface and the r -axis. Differentiating eq. (2.1.8) with respect to s yields

$$\frac{d^2 r}{ds^2} = -\frac{d\beta}{ds} \frac{dz}{ds}, \quad \frac{d^2 z}{ds^2} = \frac{d\beta}{ds} \frac{dr}{ds} \quad (2.1.9a, b)$$

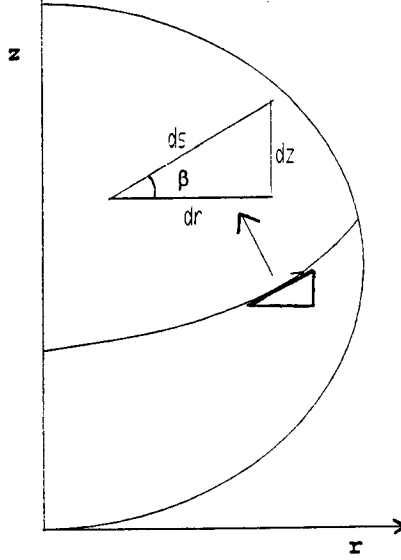


Fig. 2.2: The geometry of the Free surface [2]

Upon substitution of eq.(2.1.7) into eq.(2.1.6), with some algebraic manipulation and applying the relationships of eqs.(2.1.8a,b) and (2.1.9a,b), two differential equations , one for r and another for z ,are derived

$$\begin{aligned}\frac{d^2 r}{ds^2} &= -\frac{dz}{ds} \left\{ \pm \left[\frac{\rho}{\sigma} \Pi + \frac{c}{\sigma} \right] - \frac{1}{r} \frac{dz}{ds} \right\} \\ \frac{d^2 z}{ds^2} &= \frac{dr}{ds} \left\{ \pm \left[\frac{\rho}{\sigma} \Pi + \frac{c}{\sigma} \right] - \frac{1}{r} \frac{dz}{ds} \right\}\end{aligned}\quad (2.1.10a,b)$$

Letting $\Pi = gz - \frac{1}{2} \Omega^2 r^2$, where g is the gravitational constant and Ω is the rotational velocity, the above equations become

$$\frac{d^2 r}{ds^2} = -\frac{dz}{ds} \left\{ \pm \frac{\rho g}{\sigma} z \mp \frac{\rho \Omega^2}{2\sigma} r^2 \pm \frac{c}{\sigma} - \frac{1}{r} \frac{dz}{ds} \right\} \quad (2.1.11)$$

$$\frac{d^2 z}{ds^2} = \frac{dr}{ds} \left\{ \pm \frac{\rho g}{\sigma} z \mp \frac{\rho \Omega^2}{2\sigma} r^2 \pm \frac{c}{\sigma} - \frac{1}{r} \frac{dz}{ds} \right\} \quad (2.1.12)$$

which can be solved simultaneously, given appropriate boundary conditions, to determine the equilibrium free surface coordinates r and z .

2.2 BOUNDARY CONDITIONS AND PHYSICAL CONSTRAINTS

When integrating from the center of the vessel to the vessel wall the following initial conditions are applied

$$r(0) = \frac{dz}{ds}(0) = 0, \quad z(0) = z_o, \quad \frac{dr}{ds}(0) = 1 \quad (2.2.1)$$

In this problem the origin of the coordinate system is moved to z_o , therefore the initial conditions become

$$r(0) = z(0) = \frac{dz}{ds}(0) = 0, \quad \frac{dr}{ds}(0) = 1 \quad (2.2.2)$$

The conditions at the end point $s=s_f$ are

$$r(s_f) = r_A, \quad z(s_f) = z_A \quad (2.2.3)$$

where (r_A, z_A) is the endpoint of the free surface that is in contact with the vessel wall. The point (r_A, z_A) is referred to as the contact point.

In addition to the boundary conditions, certain physical constraints inherent to the problem must also be

satisfied. The physical constraints are dependent on the vessel geometry and the volume of the liquid filling the vessel.

No matter what the shape the free surface of the liquid may take, the condition

$$V_2 = V_1 + V \quad (2.2.4)$$

must be satisfied (see Fig. 2.3), where V is the volume of the liquid contained within the vessel. V_2 is the volume bounded by the vessel wall and the $z=z_A$ plane, which is calculated by

$$V_2 = \pi \int_0^{z_A} R^2 dz \quad (2.2.5)$$

where R is the radius of the vessel at dz . V_1 is the volume bounded by the free surface and the $z=z_A$ plane, which is calculated by

$$V_1 = \pi \int_{z_0}^{z_A} r^2 dz \quad (2.2.6)$$

where r is the distance from the axis of symmetry to the free surface.

Another condition that must also be met is at the contact point (see Fig. 2.3), given by

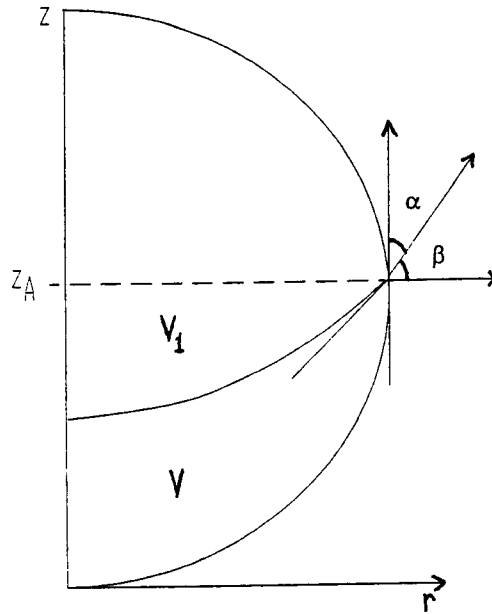


Fig. 2.3: The Physical Constraints [2]

$$\psi = \beta + \alpha \quad (2.2.7)$$

where ψ is the angle formed by the tangent to the vessel wall and the r -axis, α is the contact angle, and β is the angle formed by the tangent to the free surface and the r -axis. The contact angle α is the angle formed by the tangent to the free surface at the contact point and the plane surface of the vessel wall.

There is also a condition on the surface tension coefficient σ that must be satisfied which is the Dupre-Young condition given by

$$\sigma \cos \alpha = \sigma_{ls} - \sigma_{vs} \quad (2.2.8)$$

where σ_{ls} is the surface tension coefficient at the liquid-solid interface, and σ_{vs} is the surface tension coefficient at the vapor-solid interface. The Dupre-Young condition specifies that the contact line of a liquid and gas can be stable only if

$$|\sigma_{ls} - \sigma_{vs}| \leq \sigma \quad (2.2.9)$$

It will be assumed that this inequality is always satisfied.
(See [2] for more information)

2.3 DIMENSIONAL ANALYSIS

Upon analysis of the coefficients in eqs.(2.1.11) and (2.1.12) , their units are found to be:

$$\frac{\rho g}{\sigma} \rightarrow \left[\frac{1}{L^2} \right] \quad (2.3.1)$$

$$\frac{\rho \Omega^2}{2\sigma} \rightarrow \left[\frac{1}{L^3} \right] \quad (2.3.2)$$

$$\frac{c}{\sigma} \rightarrow \left[\frac{1}{L} \right] \quad (2.3.3)$$

Therefore, given an appropriate length scale the nondimensional coefficients will take the following forms:

$$\begin{aligned} Bo^* &= \frac{\rho g}{\sigma} L^2, \quad Ro^* = \frac{\rho \Omega^2}{2\sigma} L^3, \\ q^* &= \frac{c}{\sigma} L, \quad r^* = \frac{r}{L}, \quad z^* = \frac{z}{L} \end{aligned} \quad (2.3.4)$$

where Bo^* is the Bond number, and Ro^* is the Rotation number. A convenient length scale will be a physical length scale inherent to the problem, such as the radius of the vessel.

The Bond number is the ratio of the gravitational force to the surface tension force, and the Rotation number is the ratio of the centrifugal force to the surface tension force. The existence of these two nondimensional numbers in the free surface equations leads to the following similarity law: Whenever a unique solution exists for any two capillary surfaces possessing the same values for the Bond number, the Rotation number, and the contact angle, over geometrically similar domains, the capillary surfaces themselves will be geometrically similar [2].

With the nondimensional variables defined, the governing equations take the following nondimensional form

$$\frac{d^2 r^*}{ds^{*2}} = -\frac{dz^*}{ds^*} \left\{ z^* Bo^* - r^{*2} Ro^* + q^* - \frac{1}{r} \frac{dz^*}{ds^*} \right\} \quad (2.3.5)$$

$$\frac{d^2 z^*}{ds^{*2}} = \frac{dr^*}{ds^*} \left\{ z^* Bo^* - r^{*2} Ro^* + q^* - \frac{1}{r} \frac{dz^*}{ds^*} \right\} \quad (2.3.6)$$

with the following boundary conditions:

$$r^*(0) = \frac{dz^*}{ds^*}(0) = 0, \quad z^*(0) = 0, \quad \frac{dr^*}{ds^*}(0) = 1 \quad (2.3.7)$$

$$r^*(s_f^*) = r_A^*, \quad z^*(s_f^*) = z_A^* \quad (2.3.8)$$

The nondimensional form of the equations will be assumed throughout the rest of the work, therefore the asterisk will be dropped for notational convenience.

CHAPTER 3

SOLUTION TECHNIQUES

The development of the governing equations in chapter 2 resulted in two coupled, nonlinear, second order differential equations. Since analytical solutions to nonlinear equations do not exist at this time, they must be solved numerically. The constant q found in the governing equations and the contact point (r_A, z_A) are unknowns in the problem and must be determined as part of the solution using the physical constraints given by eqs. (2.2.4) and (2.2.7).

In this chapter, a technique developed by Slobozhanin and Tyupstov [7] for determining q and the contact point (r_A, z_A) is described. Then a numerical technique is adapted to the method in [7] to obtain a more efficient and accurate method of determining q and the contact point (r_A, z_A) .

3.1 THE GRAPHICAL METHOD

The technique of interest for determining the shape of the free surface is a graphical method developed by L.A. Slobozhanin and A.D. Tyuptsov [7]. The graphical method

derives its name from the procedure of obtaining information from graphs of functions or data in order to determine the contact point.

In order to determine the contact point (r_A, z_A) , the graphical method integrates eqs. (2.3.5) and (2.3.6) along the free surface until a point (r, z) is found that satisfies the physical constraints eqs. (2.2.4) and (2.2.7). But, analytical solutions for $\beta(r)$ and $V_1(r)$ are not known, therefore the differential equations

$$\frac{d\beta}{ds} = zBo - r^2 Ro + q - \frac{1}{r} \frac{dz}{ds} \quad (3.1.1)$$

$$\frac{dV_1}{ds} = \pi r^2 \frac{dz}{ds} \quad (3.1.2)$$

, subject to the following initial conditions:

$$\beta(0) = 0, V_1(0) = 0 \quad (3.1.3a, b)$$

must be integrated along with eqs. (2.3.5) and (2.3.6) to obtain the curves $\beta(r)$ and $V_1(r)$. Since q is an unknown constant a family of curves for $\beta(r, q)$ and $V_1(r, q)$ can be calculated for different values of q .

If a dense family of curves are plotted for $\beta(r)$ and are plotted along with the curve $\psi(r) - \alpha$, a curve C_1 can be

constructed from all the possible points (r,q) that satisfy (see Figures 3.1 and 3.2)

$$\beta(r,q) = \psi(r) - \alpha \quad (3.1.4)$$

Also, if the curves $V_1(r,q)$ are plotted along with the curve $V_2(r) - V$ (see Fig. 3.3), a second curve C_2 can be constructed from all the possible points (r,q) that satisfy (see Fig. 3.4)

$$V_1(r,q) = V_2(r) - V \quad (3.1.5)$$

When the curves C_1 and C_2 are plotted together (see Fig. 3.5), their intersection point (q_A, r_A) defines a point on the vessel wall and a value q that satisfies both physical constraints eqs. (2.2.4) and (2.2.7). Therefore, with q and (r_A, z_A) known the governing equations can be integrated with fully specified boundary conditions, and q to obtain the free surface coordinates.

In the case where more than one intersection point (q_A, r_A) exists for C_1 and C_2 , each point must be evaluated to determine if the free surface associated with that point is physically possible (i.e. lies within the vessel, ends at the vessel wall).

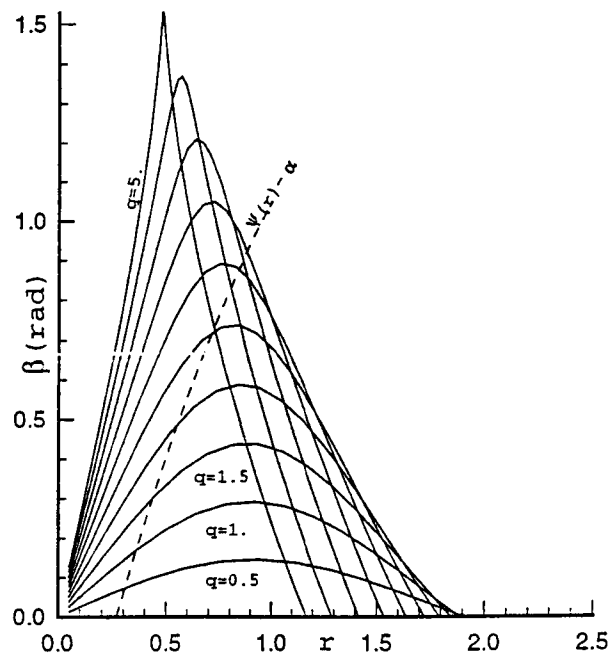


Fig. 3.1: Family of $\beta(r)$ curves for different values of q . The dashed curve is the curve $\psi(r)-\alpha$.

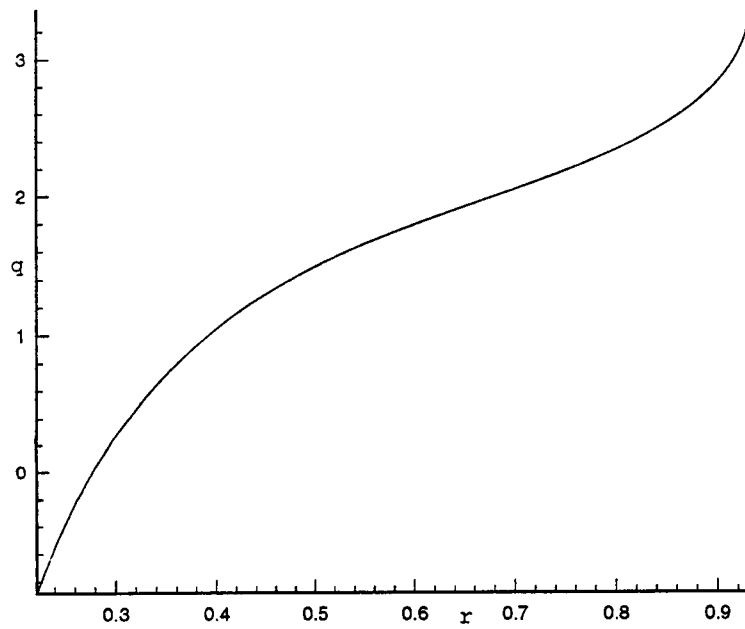


Fig. 3.2: Plot of C_1

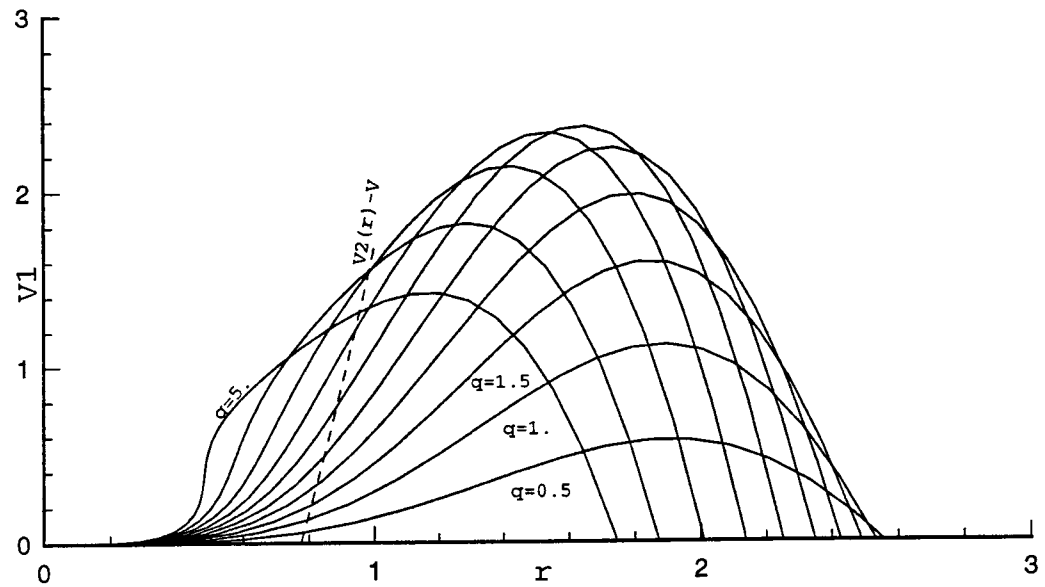


Fig. 3.3: Family of $V_1(r)$ for different values of q .
The dashed curve is the curve $V_2(r)-V$.

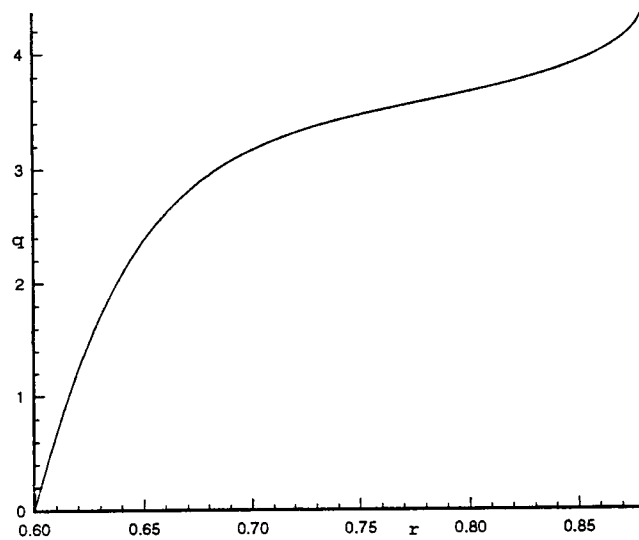


Fig. 3.4: Plot of C_2

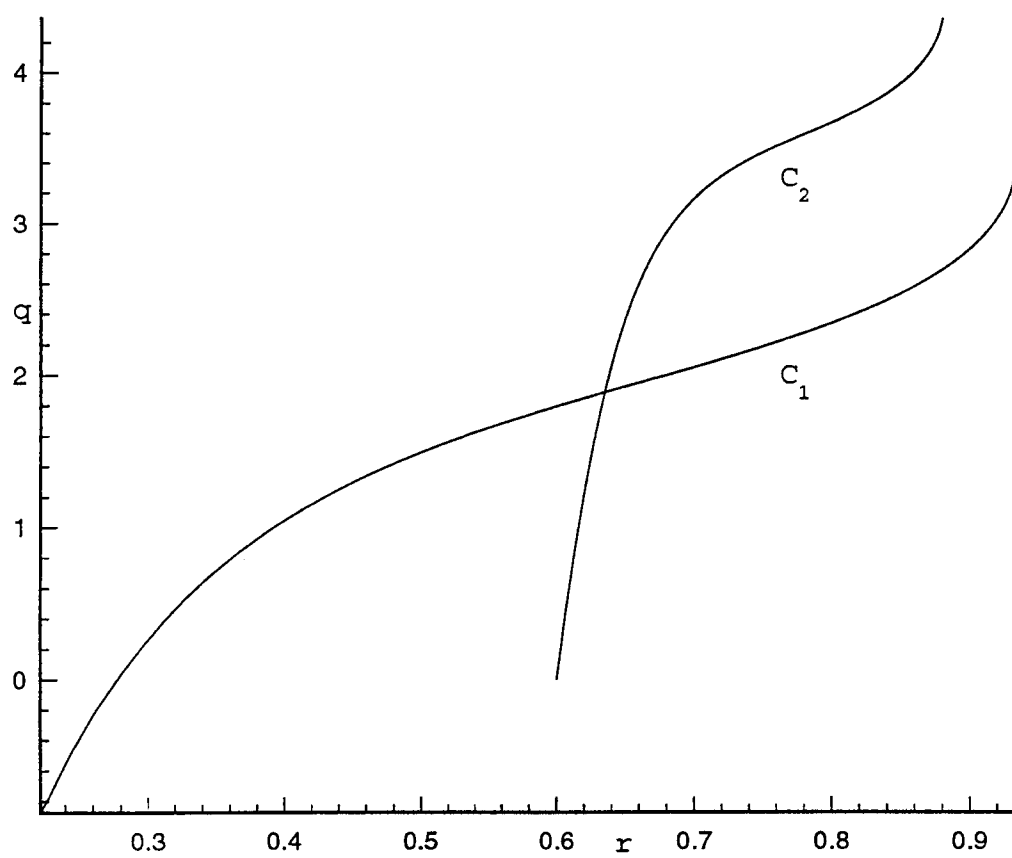


Fig. 3.5: Plot of C_1 and C_2 .

3.2 A NUMERICAL SOLUTION

Because the graphical method finds the solution through the use of curve plotting, it lacks the ability to find an accurate solution. The reason for the lack of accuracy is due to the fact that one can only plot and analyze a finite number of curves, therefore a more accurate solution may be over looked. Implementing the graphical method numerically would allow a solution to be obtained more efficiently and accurately without the task of plotting numerous curves. Since the graphical method determines the solution from the intersection of curves, it would appear to be a good candidate for numerical assessment by implementing a root finding method.

In order to obtain the contact point, a solution (r_A, q_A) must be found that satisfies both of the physical constraints

$$\begin{aligned}\psi(r) &= \alpha + \beta(r, q) \\ V_2(r) &= V + V_1(r, q)\end{aligned}\tag{3.2.1a,b}$$

The root finding methodology that will be used to find the solution will be the Newton-Raphson method for a system of

equations. An initial guess for r_A and q_A will be updated by δr and δq given by the following equation in matrix form

$$\begin{bmatrix} \delta r \\ \delta q \end{bmatrix} = -[J]^{-1} \begin{bmatrix} F(r_A, q_A) \\ G(r_A, q_A) \end{bmatrix} \quad (3.2.3)$$

where

$$\begin{aligned} F(r, q) &= \psi(r) - \alpha - \beta(r, q) \\ G(r, q) &= V_2(r) - V - V_1(r, q) \end{aligned} \quad (3.2.4a, b)$$

and J is the Jacobian given by

$$\begin{bmatrix} \frac{\partial F}{\partial r} & \frac{\partial F}{\partial q} \\ \frac{\partial G}{\partial r} & \frac{\partial G}{\partial q} \end{bmatrix} \quad (3.2.5)$$

3.3 THE NUMERICAL PROCEDURE

To implement the root finding method the elements on the right-hand side of eq.(3.2.3) need to be determined in order to calculate δr and δq . The following describes the method for calculating the necessary data for the Newton-Raphson technique.

The computational procedure begins by numerically integrating the following set of equations

$$\frac{d^2 r}{ds^2} = -\frac{dz}{ds} \left[zBo - r^2 Ro + q - \frac{1}{r} \frac{dz}{ds} \right] \quad (3.3.1)$$

$$\frac{d^2 z}{ds^2} = \frac{dr}{ds} \left[zBo - r^2 Ro + q - \frac{1}{r} \frac{dz}{ds} \right] \quad (3.3.2)$$

$$\frac{d\beta}{ds} = zBo - r^2 Ro + q - \frac{1}{r} \frac{dz}{ds} \quad (3.3.3)$$

$$\frac{dV_1}{ds} = \pi r^2 \frac{dz}{ds} \quad (3.3.4)$$

forward along the equilibrium free surface line from $s=0$ to $s=s_f$ for a particular value of q . The numerical integration is carried out using an initial value, third order, variable step Runge-Kutta method for a system of equations (see [6]). To apply the Runge-Kutta method to the equations, the second order differential equations (3.3.1) and (3.3.2) must be reduced to first order differential equations. After a reduction of order is carried out on eq.(3.3.1) and eq.(3.3.2), the system of equations become

$$u_1 = r \quad \frac{du_1}{ds} = u_2 \quad (3.3.5)$$

$$u_2 = \frac{dr}{ds} \quad \frac{du_2}{ds} = \frac{d^2 r}{ds^2} \quad (3.3.6)$$

$$u_3 = z \quad \frac{du_3}{ds} = u_4 \quad (3.3.7)$$

$$u_4 = \frac{dz}{ds} \quad \frac{du_4}{ds} = \frac{d\beta}{ds} \quad (3.3.8)$$

$$u_5 = \beta \quad \frac{du_5}{ds} = \frac{d\beta}{ds} \quad (3.3.9)$$

$$u_6 = V_1 \quad \frac{du_6}{ds} = \frac{dV_1}{ds} \quad (3.3.10)$$

These equations are integrated forward using the following boundary conditions

$$u_1(0) = u_3(0) = u_4(0) = 0, \quad u_2(0) = 1 \quad (3.3.11)$$

$$u_1(s_f) = r_A, \quad u_3(s_f) = z_A \quad (3.3.12)$$

Two problems occur using the initial value integrator:

(a) Equations (3.3.1) and (3.3.2) are singular at $s=0$

because of the $\frac{1}{r} \frac{dz}{ds}$ term in each equation. To overcome the singularity problem [6] suggests using the following asymptotic expansions near $s=0$,

$$r = s - \frac{1}{24} q^2 s^3 + \frac{1}{40} \left(Ro - \frac{1}{4} Bo q^2 + \frac{1}{48} q^4 \right) s^5 + \dots \quad (3.3.13)$$

$$z = \frac{1}{4} q^2 s + \frac{1}{16} \left(-Ro + \frac{1}{16} Bo q - \frac{1}{48} q^3 \right) s^4 + \dots \quad (3.3.14)$$

which is valid in a small neighborhood about the point $s=0$.

(b) The length of the equilibrium free surface line is not known *a priori*, therefore the end point $s=s_f$ at the vessel wall is unknown. This problem is corrected by updating s_f

with a Newton-Raphson method for a single equation. The initial guess for s_f is r_0 and is updated by δs_f given by

$$\delta s_f = -\frac{(r-r_A)}{\frac{dr}{ds}} \quad (3.3.15)$$

where r is the value calculated at the previous end point.

From the data obtained after integration, $F(r_A, q_A)$ and $G(r_A, q_A)$ are calculated. With $F(r_A, q_A)$ and $G(r_A, q_A)$ known, the elements of the Jacobian need to be calculated. Because $F(r, q)$ and $G(r, q)$ are determined numerically, an analytical expression for the partial derivatives can not be obtained. Therefore, the partial derivatives are calculated using finite difference approximations. For example, a second order central difference approximation for $\frac{\partial F}{\partial r}$ and $\frac{\partial F}{\partial q}$ would be given by

$$\frac{\partial F(r_A, q_A)}{\partial r} = \frac{F(r_A + \Delta r, q_A) - F(r_A - \Delta r, q_A)}{2\Delta r} \quad (3.3.16)$$

$$\frac{\partial F(r_A, q_A)}{\partial q} = \frac{F(r_A, q_A + \Delta q) - F(r_A, q_A - \Delta q)}{2\Delta q} \quad (3.3.17)$$

Because an approximation is used to calculate the derivatives the numerical method is a quasi-Newton's method (see [3]).

So, numerical integration must be carried out for the initial point and for each point needed to calculate the derivatives.

After calculating the Jacobian and the inverse Jacobian, r_A and q_A are updated by δr and δq calculated using eq.(3.2.3) until $\delta r = \delta q = 0$ or if δr and δq are within some specified tolerance.

After r_A and q_A are found, eqs (3.3.1) and (3.3.2) are integrated with q_A and fully specified boundary conditions given by the contact point (r_A, z_A) to obtain the free surface coordinates.

3.4 CALCULATION STEPS

In summary, the numerical procedure is carried out by following the steps below:

- (1) Input Bo and Ro , or input the information to calculate Bo and Ro .
- (2) Input the liquid fill level
- (3) Input initial guess for r_A and q_A .
- (4) Set Δr and Δq for calculating derivatives.
- (5) Perform integration for each point.

- (6) Calculate $\psi(r)$ and $V_1(r)$ for each point based upon the geometry of the vessel.
- (7) Calculate $F(r_A, q_A)$ and $G(r_A, q_A)$ for each point.
- (8) Calculate the Jacobian.
- (9) Calculate the inverse Jacobian.
- (10) Calculate δr and δq .
- (11) Check the tolerance of δr and δq .
- (12) If the tolerance is not satisfied
 - (12a) Update r_A and q_A .
 - (12b) Repeat steps 4-11
- (13) If tolerance is satisfied: Eqs. (2.3.3) and (2.3.4) are integrated with q_A and the calculated boundary condition to obtain the free surface.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 COMPARISON OF THE NUMERICAL METHOD TO OTHER RESULTS

In [7], Slobozhanin and Tyupstov illustrate the graphical method with the following example:

An elongated ellipsoidal vessel with semimajor and minor lengths 100 cm and 50 cm, respectively, partially filled with a liquid of density $\rho = 1 \text{ gm/cm}^3$ and whose coefficient of surface tension $\sigma = 49.05 \text{ dyne/cm}$, having a contact angle $\alpha = 30^\circ$. The liquid volume comprises 10% of the total volume. The vessel is not rotating, the z axis is directed away from the liquid towards the gas, and the system is subject to a uniform gravity field in the opposite direction and is of magnitude 0.07848 cm/s^2 .

Using the semiminor length as the length scale and the information presented in the example, the following nondimensional values are calculated:

(A) the semimajor and minor lengths: $H = 2$, $W = 1$

(B) the volume of the ellipsoid: $V_{el} = 8.378$

(C) the volume of the liquid: $V = 0.8378$

(D) the Bond number: $Bo = 4$

(E) the Rotation number: $Ro = 0$

Also, $\psi(r)$ and $V_2(r)$ are given analytically in [7], and are

$$\psi(r) = \pm \frac{W}{Hr_A} \sqrt{W^2 - r^2} \quad (4.1.1)$$

$$V_2(r) = \frac{2}{3} \pi W H \left(W \mp \sqrt{W^2 - r^2} \right) \quad (4.1.2)$$

where the upper sign corresponds to the lower half of the ellipsoid and the lower sign to the upper half.

The results obtained from the graphical method are presented in the following Table I.

TABLE I: Graphical Method Results

POINT	q	rA (cm)	zA (cm)	dzA (cm)
1	23.5	31.86	77.07	9.43
2	54	43.75	48.41	61.45

The graphical method was able to determine two possible contact points for the conditions given in the example. After testing each point, [7] found that point 2 did not represent a physically possible free surface. The

nonphysical point can be determined by taking the difference

$$z_o = z_A - \Delta z_A \quad (4.1.3)$$

For point 2, $z_o = -13.04$ cm . Since the bottom of the vessel lies on the origin of the coordinate system, z_o for point 2 places the free surface below the vessel.

The example solved in [7], was used to check the numerical method developed in chapter 3. The results obtained by the numerical method are given in Table II.

TABLE II: Numerical Method Results

POINT	q	rA(cm)	zA(cm)	dzA(cm)
1	1.88	31.75	77.26	9.19
2	4.26	43.86	47.96	61.03

Two possible contact points were also obtained using the numerical method. Though the values for q are different, the coordinates for the contact point are in relatively good agreement with the results obtained by the graphical method. The numerical method also predicted the nonphysical point.

The analytical expression for $V_2(r)$ given in [7] was found to be erroneous. Upon verification of $V_2(r)$ by

integrating eq.(2.2.5), the analytical expression was calculated as

$$V_2(r) = \frac{2}{3} \pi W H \left(W \mp \frac{2W^2 + r^2}{2W^2} \sqrt{W^2 - r^2} \right) \quad (4.1.4)$$

not as given in [7]. Using the corrected expression for $V_2(r)$ and the conditions of the example, the contact point is calculated as $r_A = 42.57$ cm and $z_A = 47.53$ cm for $q = 1.21$, and the free surface is shown in Figure 4.1.

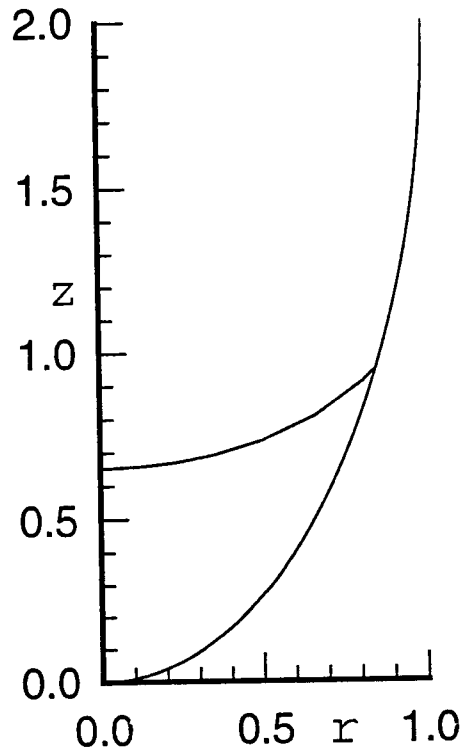


Fig. 4.1: Free surface calculated for example in [8] with the correct volume.

Concus in [4] used a variable-step size, fourth order Adams-Moulton method to integrate the governing equations for a cylindrical vessel. In [4] only a change in Bond number is taken into account in the free surface calculations. The free surface results obtained in [4] for a contact angle $\alpha = 30^\circ$ is shown in Fig. 4.2. The results obtained by the numerical method are shown in Fig. 4.3. Though Concus did not specify the values for the contact points, it is observed that the free surface shapes obtained from the numerical method follow the same pattern for increasing Bond number that is shown in [4].

Figure 4.4 shows the equilibrium free surface for liquid fill volume $V=30\%$ with a contact angle $\alpha = 60^\circ$. The Bond number is 2 and the Rotation number is 10. Figure 4.6 shows the equilibrium free surface for liquid fill volume $V=70\%$ with a contact angle $\alpha = 120^\circ$. The Bond number is 1 and the Rotation number is 5. In both cases, the vessel is an ellipsoid with semi-axes ratio 1:2. Figures 4.4 and 4.6 were obtained from [2]. Figures 4.5 and 4.7 are the free surfaces obtained from the numerical method for the same conditions given in [2]. Again it is observed that the results obtained

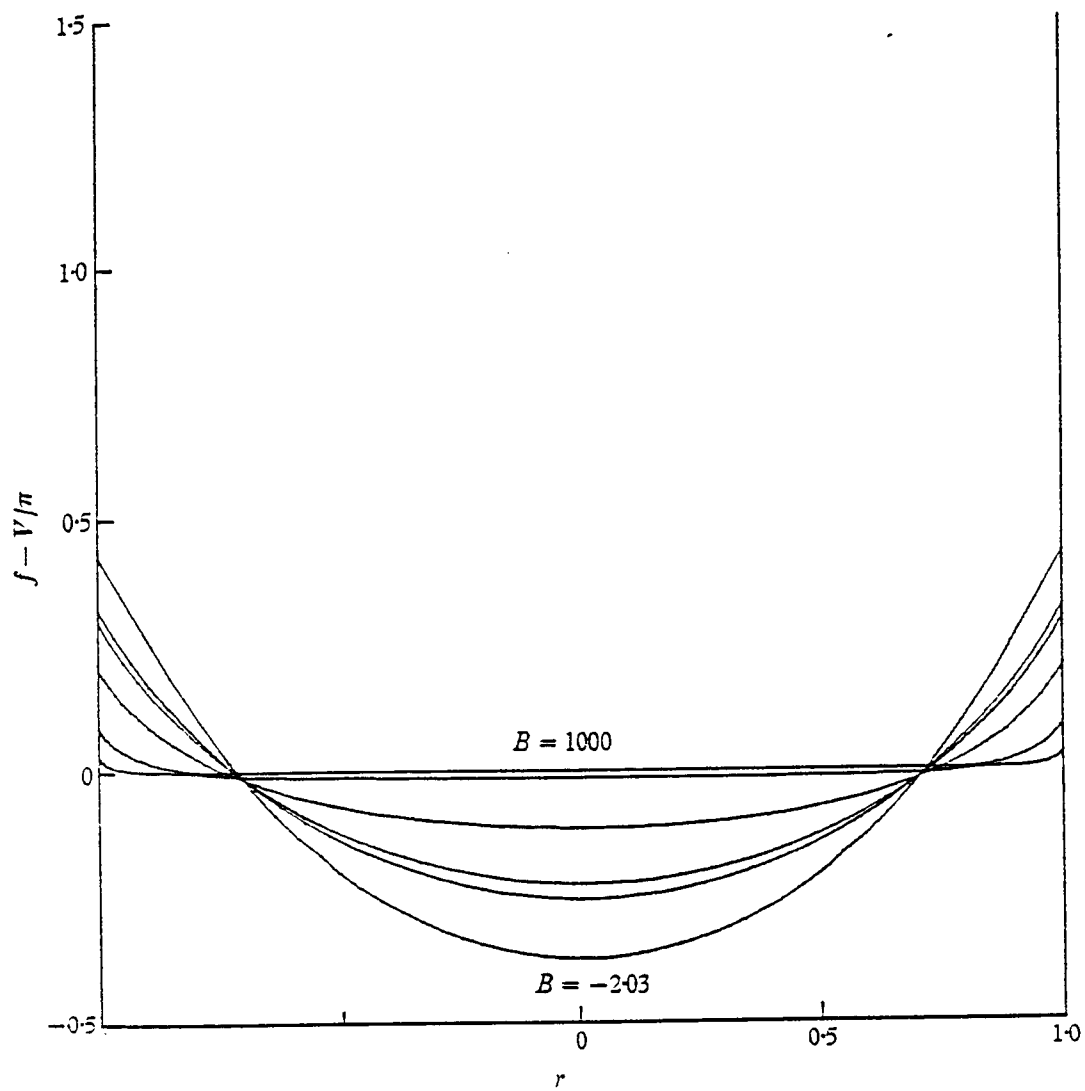


Fig. 4.2: Free Surfaces for $\alpha = 30^\circ$ and different Bo 's, obtained from [4].

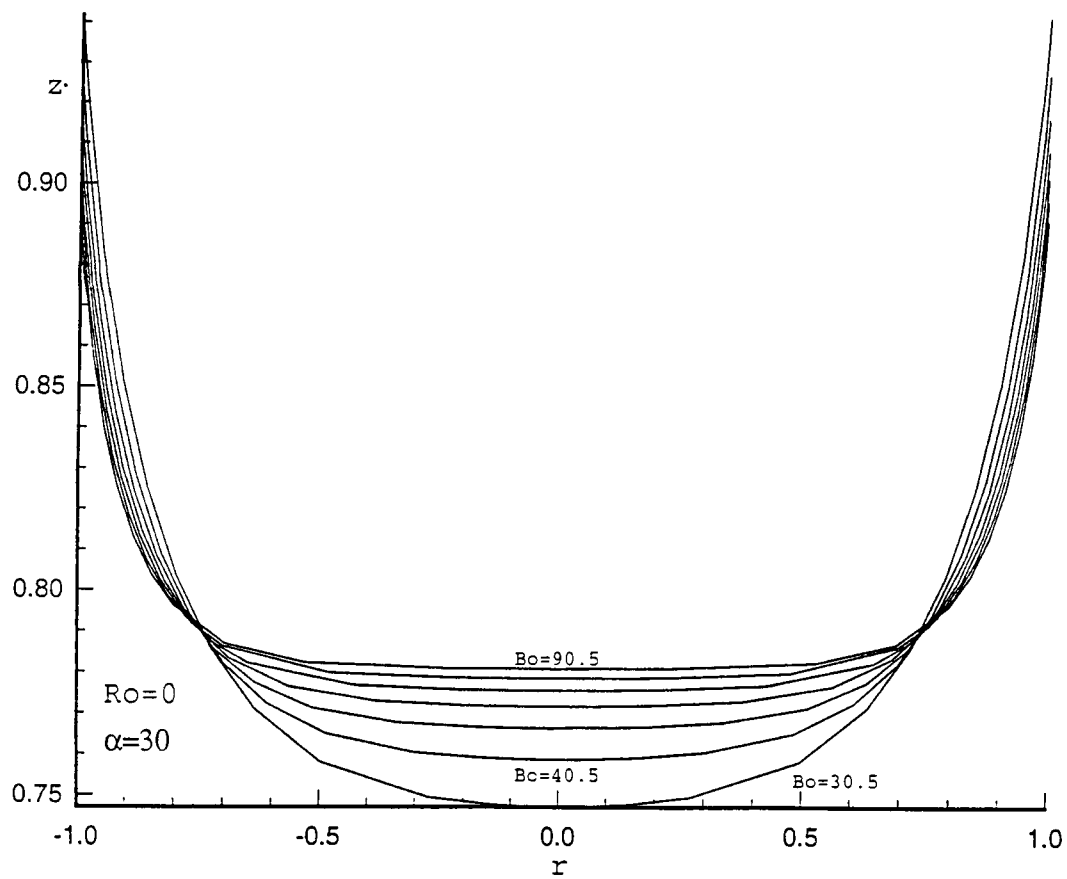


Fig. 4.3: Free Surfaces obtained by the numerical method for a cylinder, $\alpha = 30^\circ$ and different Bo 's.

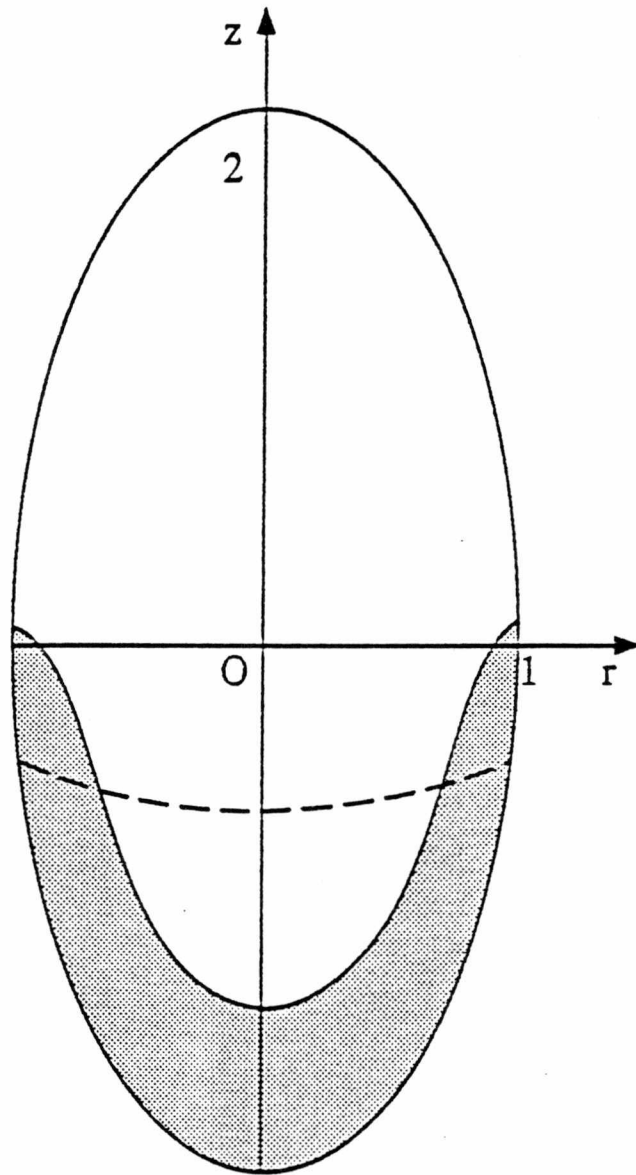


Fig. 4.4: Free Surfaces obtained from [2] for $V=30\%$, $\alpha = 60^\circ$, $Bo=2$, $Ro=0$ (the dashed line) and $Ro=10$.

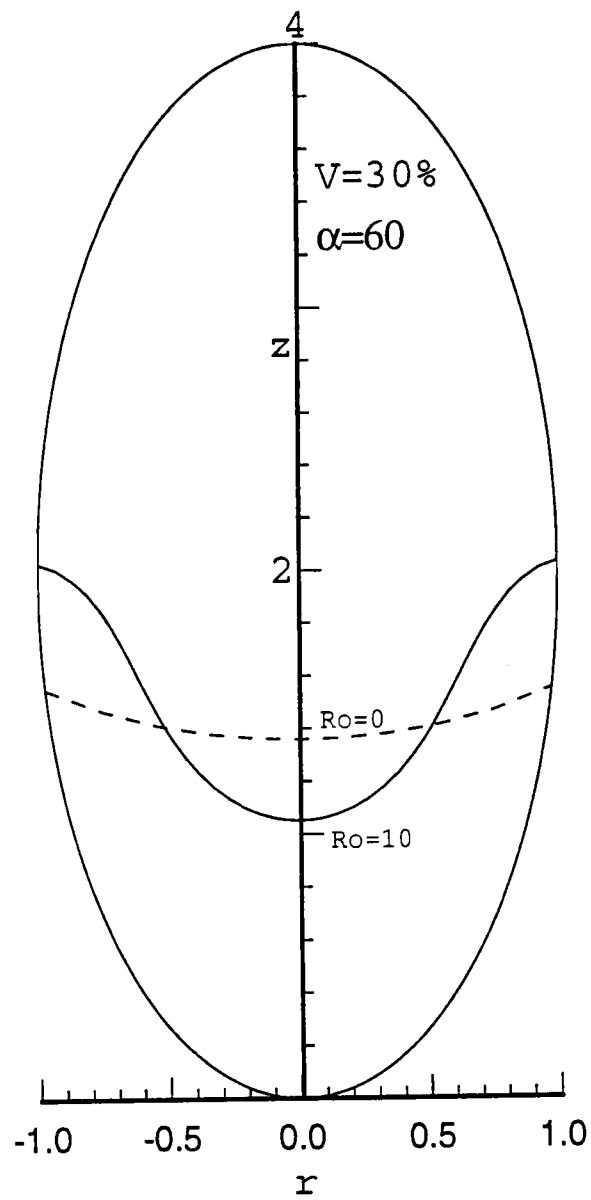


Fig. 4.5: Free surfaces obtained from numerical method for $V=30\%$, $\alpha = 60^\circ$, $Bo=2$, $Ro=0$ and $Ro=7$.

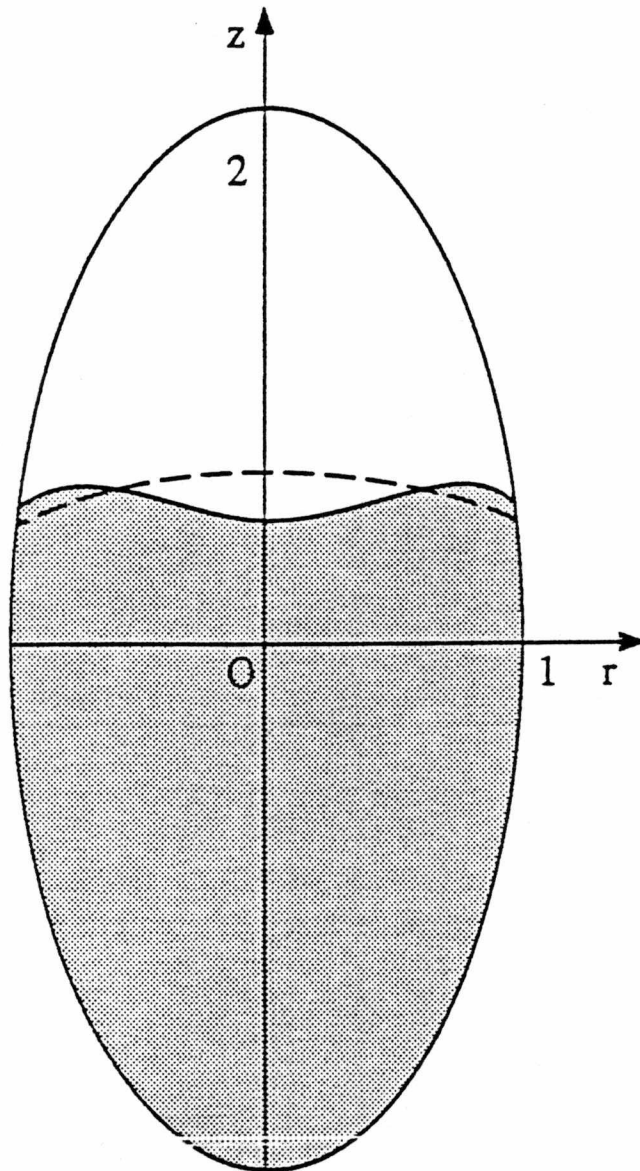


Fig. 4.6: Free Surfaces shown in [2] for $V=70\%$, $\alpha=120^\circ$, $Bo=1, Ro=0$ (the dashed line) and $Ro=5$.

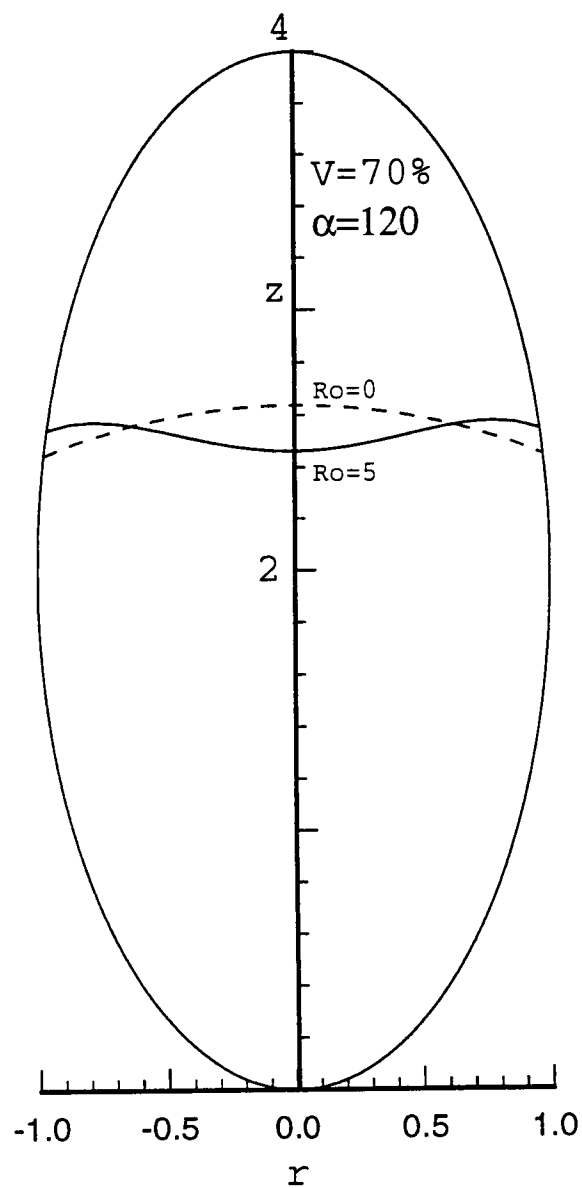


Fig. 4.7: Free Surfaces obtained by the numerical method for $V=70\%$, $\alpha=120^\circ$, $Bo=1$, $Ro=0$ and $Ro=5$.

from the numerical method follow the same free surface pattern as the free surfaces shown in [2].

4.2 RESULTS OBTAINED FROM THE NUMERICAL METHOD

Presented are some the free surfaces calculated for a liquid contained in three vessel geometries for two conditions. The vessel geometries are: the ellipsoid given in the example, the sphere, and the cylinder. The conditions examined are: (1) increasing Bond number without rotation, and (2) constant Bond number with increasing Rotation number. Along with each figure, a table is presented that lists the calculated nondimensional values for the stated conditions.

A. THE ELLIPSOID

The calculations were made for an ellipse with semimajor and minor lengths 100 cm and 50 cm, respectively.

Figure 4.8 is the equilibrium free surface lines associated with two different Bond numbers for a liquid with a contact angle $\alpha = 30^\circ$ and that fills 30% of the vessel. The solid line is the free surface for $Bo=60$ and the dashed line

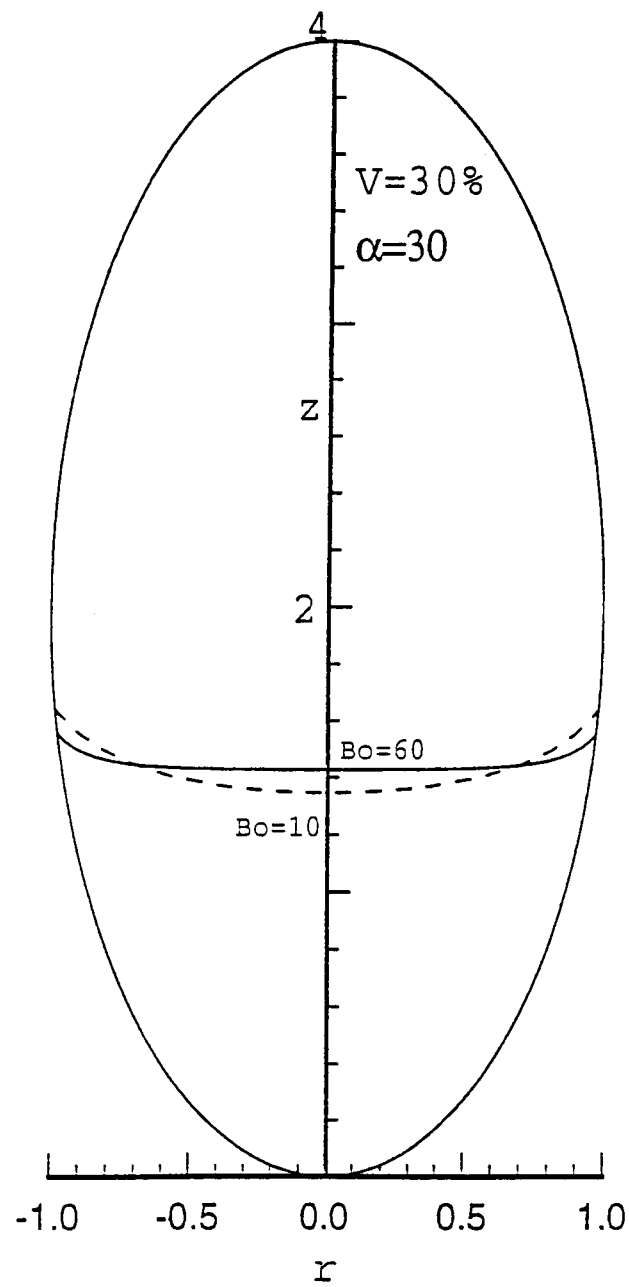


Fig. 4.8: Ellipsoid for $\alpha=30^\circ$, $Bo=10$ and $Bo=60$, $Ro=0$ is the free surface for $Bo=10$.

Table III lists the calculated parameters for the different Bond numbers.

Figure 4.9 is a plot of the free surfaces for each Bond number presented in Table III. The free surfaces are plotted without the vessel boundary to show the detail of the behavior of the free surfaces as the Bond number increases.

Figure 4.10 is the free surfaces associated with various Rotation numbers for $Bo=2$. The liquid contact angle is $\alpha=30^\circ$ and the fill level is 30%. The dashed curve is the free surface for $Ro=0$. Table IV lists the calculated values for the different Rotation numbers.

Figure 4.11 is the free surface plots of a liquid with contact angle $\alpha=120^\circ$, and 70% fill level. The dashed curve is for $Bo=1$ and $Ro=0$. Table V lists the calculated values for each Rotation number.

TABLE III: Values for ellipsoid with $\alpha=30^\circ$, $Ro=0$

Bo	Ro	q	za	ra	ψ	β	v2	v1
10	0	0.5623	1.6399	0.9837	1.4795	0.9559	3.0697	0.5565
20	0	0.2489	1.6029	0.9801	1.4696	0.9463	2.9578	0.4445
30	0	0.1246	1.5823	0.9779	1.4644	0.9408	2.8956	0.3823
40	0	0.0672	1.5686	0.9765	1.4608	0.9372	2.8544	0.3411
50	0	0.0383	1.5586	0.9753	1.4581	0.9345	2.8245	0.3112
60	0	0.0229	1.5509	0.9745	1.4561	0.9325	2.8015	0.2882

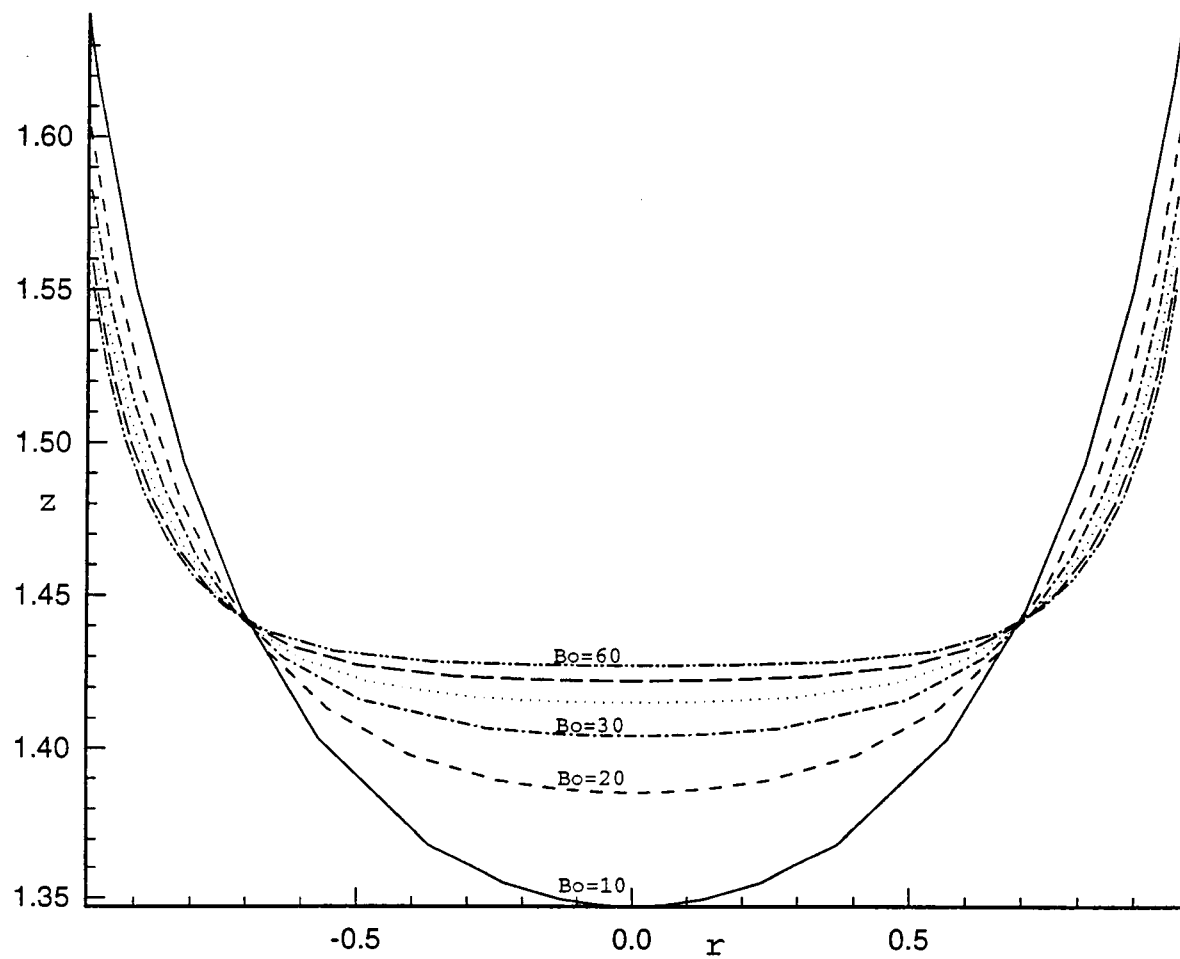


Fig. 4.9: Free surfaces for the Bond numbers given in Table III

TABLE IV: Values for ellipsoid with $\alpha = 30^\circ$ and $Bo=2$

Bo	Ro	q	zA	rA	ψ (rad)	β (rad)	V2	V1
2	0	1.287	1.7112	0.990	1.498	0.975	3.2877	0.7745
2	1	1.692	1.7492	0.992	1.5077	0.984	3.405	0.8917
2	2	2.093	1.7946	0.995	1.5192	0.996	3.5457	1.0325
2	3	2.485	1.8506	0.997	1.5334	1.010	3.7203	
2	4	2.862	1.9222	0.999	1.5513	1.028	3.9445	1.4312
2	5	3.215	2.0158	1.000	1.5747	1.051	4.2383	1.725
2	6	3.531	2.1353	0.998	1.6047	1.081	4.6131	2.0998
2	7	3.806	2.2729	0.991	1.6396	1.116	5.0408	2.5276

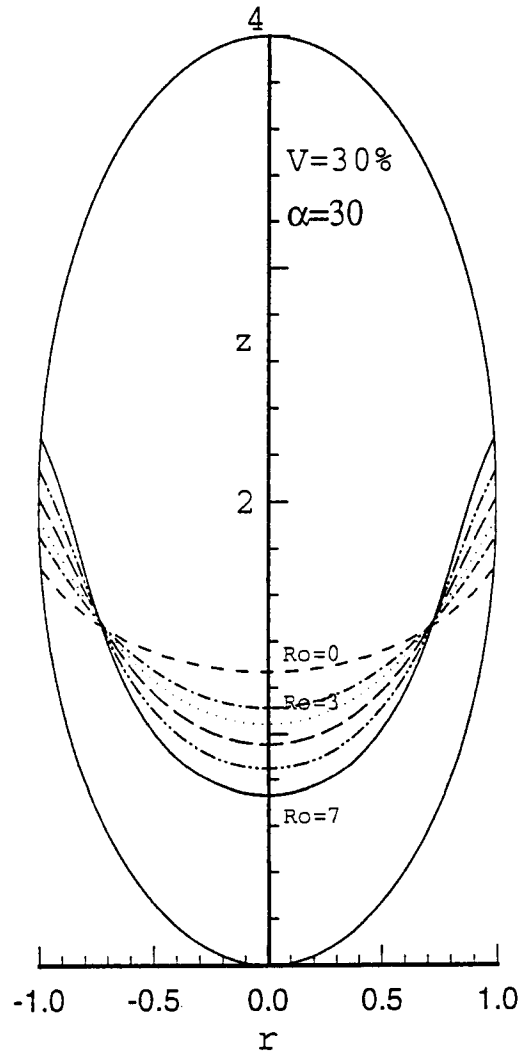


Fig. 4.10: Ellipsoid for $\alpha = 30^\circ$, $Bo=2$ and $Ro=0$ to $Ro=7$

TABLE V: Values for ellipsoid with $\alpha=120^\circ$ and $Bo=1$

Bo	Ro	q	za	ra	ψ (rad)	b(rad)	V2	V1
1	0	-0.725	2.447	0.975	1.685	-0.409	5.571	-0.294
1	1	-0.281	2.469	0.972	1.691	-0.404	5.634	-0.23
1	2	0.159	2.489	0.970	1.696	-0.398	5.693	-0.171
1	3	0.595	2.508	0.977	1.701	-0.393	5.749	-0.115
1	4	1.026	2.526	0.965	1.706	-0.388	5.803	-0.061
1	5	1.453	2.544	0.962	1.711	-0.383	5.856	-0.008
1	6	1.874	2.562	0.960	1.716	-0.378	5.908	0.044

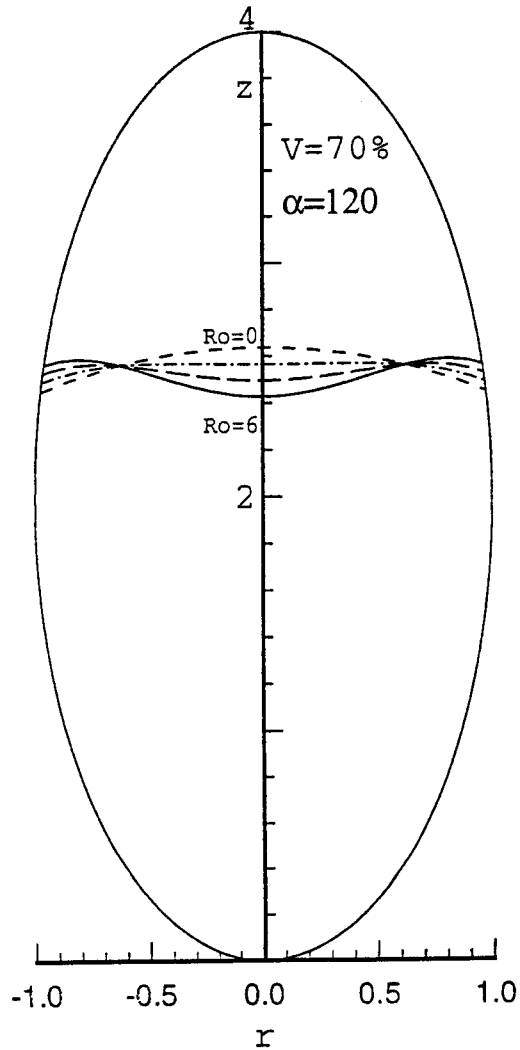


Fig. 4.11: Ellipsoid for $\alpha=120^\circ$, $Bo=1$ and $Ro=0$ to $Ro=6$

Figure 4.12 is the plot of the free surfaces for each Rotation number listed in Table V. The free surfaces are plotted without the vessel boundary to enhance the detail of the behavior of the free surface as the Rotation number increases.

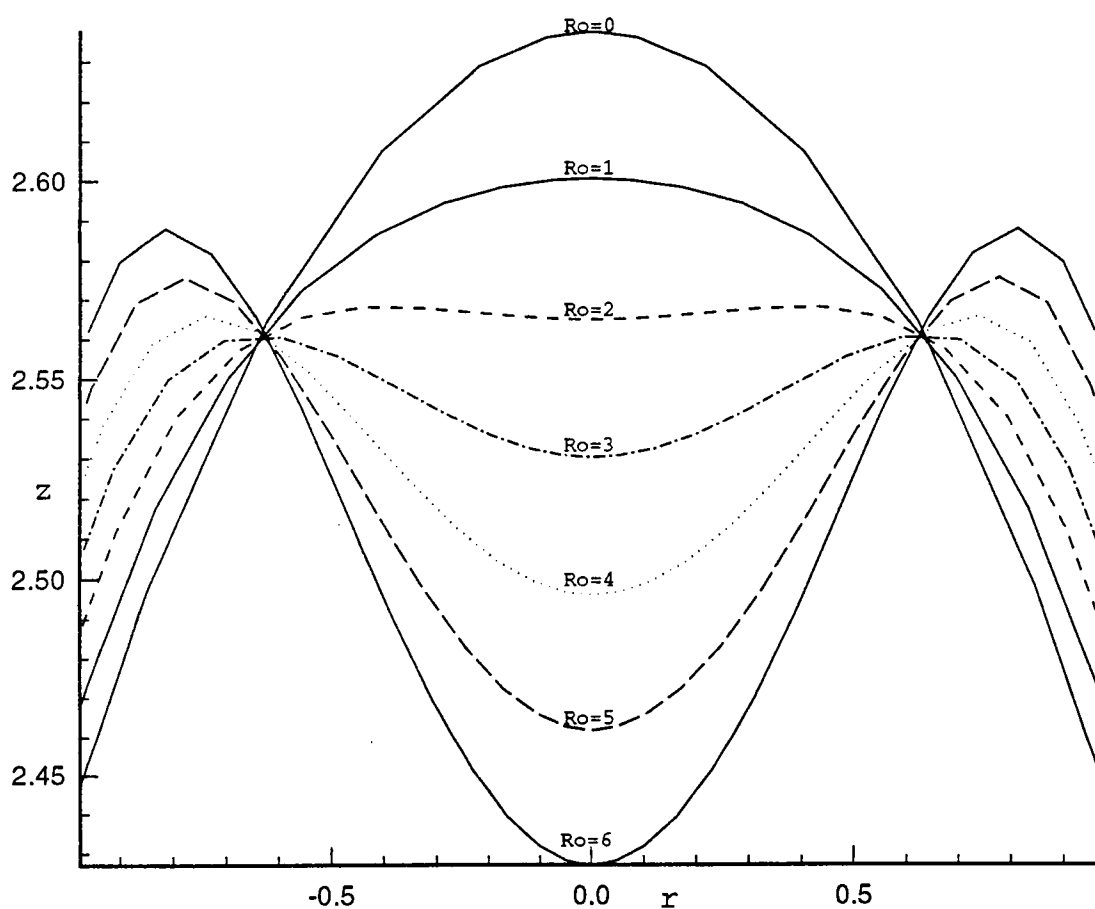


Fig. 4.12: Free surfaces for each Rotation number given in Table V.

B. THE SPHERE

Figure 4.13 is a plot of the free surface for various Bond numbers. The liquid has a contact angle $\alpha = 120^\circ$, and fills 30% of the vessel. Table VI lists the calculated values for the different Bond numbers.

TABLE VI: Values for a sphere with $\alpha = 120^\circ$ and $Ro=0$

Bo	Ro	q	zA	rA	$\psi(\text{rad})$	$\beta(\text{rad})$	V2	V1
5.5	0	-1.11	0.5361	0.8859	1.0884	-1.006	0.7415	-0.515
10.5	0	-0.70	0.5622	0.8991	1.1176	-0.977	0.8068	-0.45
20.5	0	-0.32	0.5923	0.9131	1.1508	-0.944	0.8845	-0.372
30.5	0	-0.16	0.61	0.9208	1.1702	-0.924	0.9314	-0.325
40.5	0	-0.86	0.6221	0.9259	1.1833	-0.911	0.9637	-0.293
50.5	0	-0.05	0.631	0.9294	1.1929	-0.902	0.9878	-0.269
60.5	0	-2.95	0.6379	0.9322	1.2003	-0.894	1.0067	-0.25
70.5	0	-0.02	0.6435	0.9343	1.2063	-0.888	1.0219	-0.235
80.5	0	-0.01	0.6482	0.9361	1.2113	-0.883	1.0347	-0.222

Figure 4.14 is the free surfaces plotted for $Ro=0$ to $Ro=5$ with $Bo=1$. The liquid has a contact angle $\alpha = 120^\circ$ and fills 70% of the vessel. Table VII lists the contact points and values of q for each Rotation number.

TABLE VII: Sphere with $\alpha = 120^\circ$ and $Bo=1$

Bo	Ro	q	zA	rA
1	0	-0.058	1.1931	0.9812
1	1	-0.012	1.2195	0.9756
1	2	0.3682	1.2435	0.9699
1	3	0.8266	1.2658	0.964
1	4	1.2727	1.2868	0.9581
1	5	1.7062	1.3068	0.9518

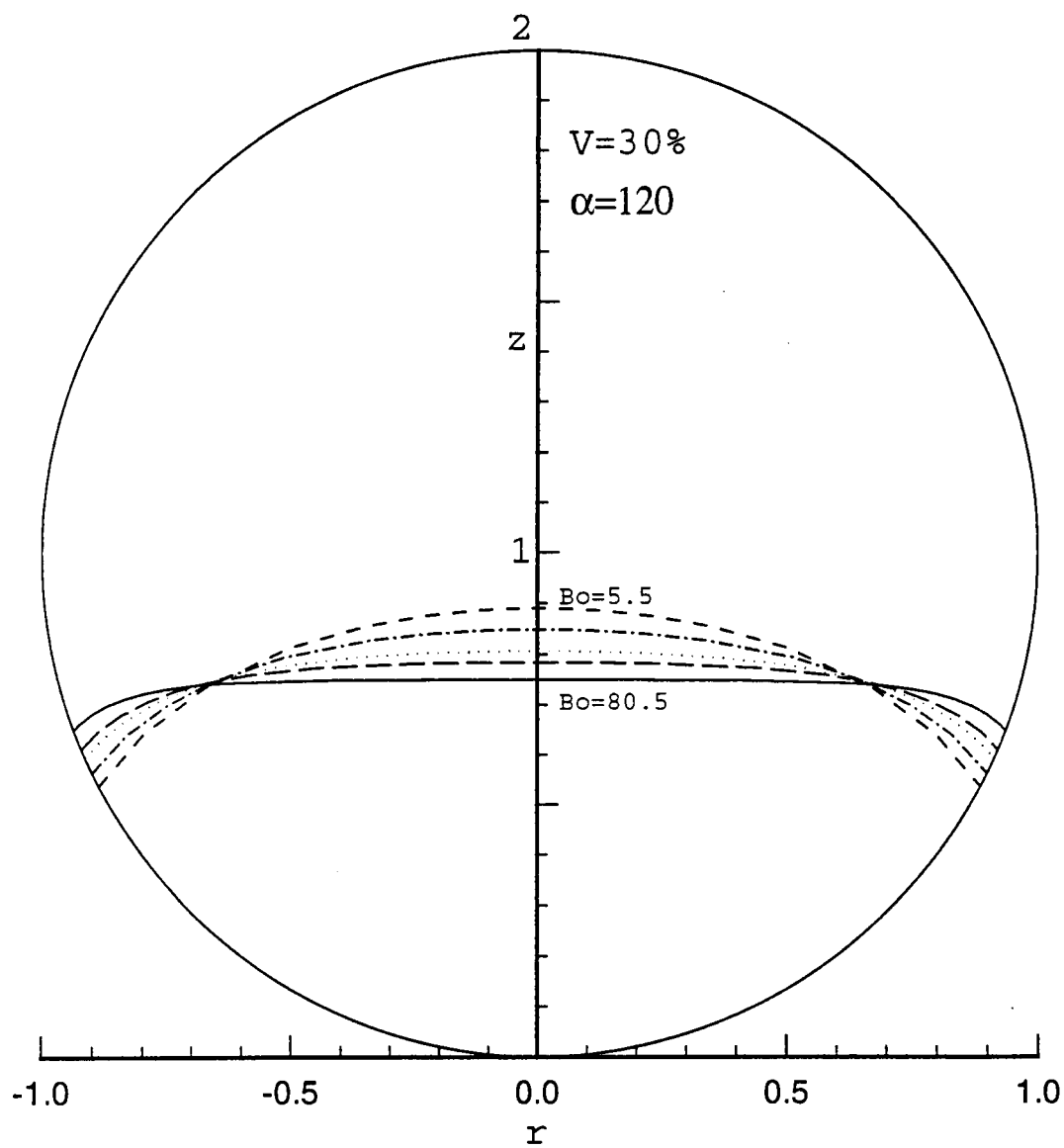


Fig. 4.13: Sphere for $\alpha=120^\circ$, $Ro=0$, and $Bo=5.5$ to $Bo=80.5$

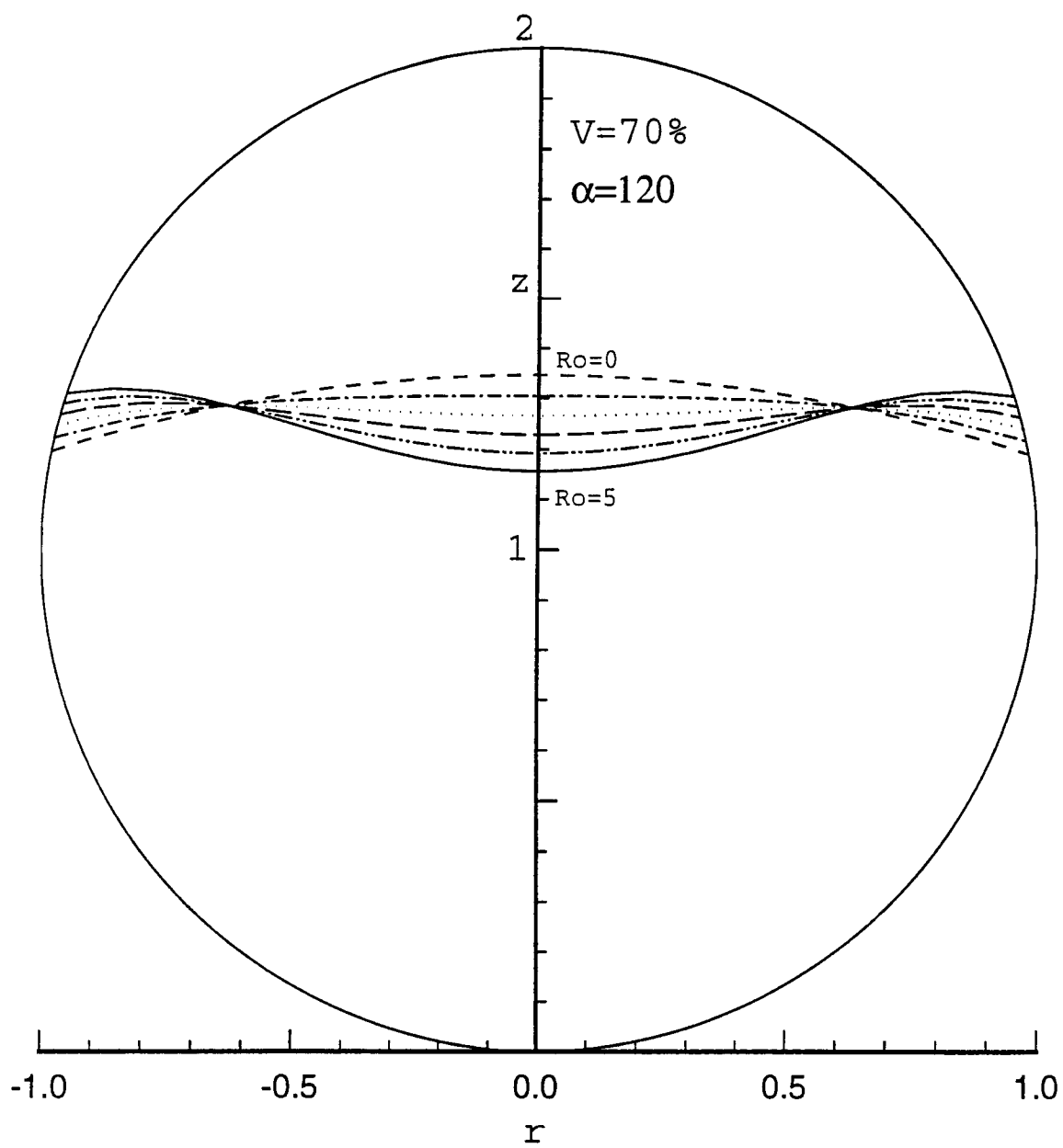


Fig. 4.14: Sphere for $\alpha=120^\circ$, $Bo=1$, and $Ro=0$ to $Ro=6$

C. THE CYLINDER

Figure 4.15 is the free surface plots for increasing values of Bond number. The liquid has a contact angle $\alpha = 30^\circ$. Table VIII lists the calculated values for each Bond number.

TABLE VIII: Values for Cylinder with $\alpha = 30^\circ$ and $Ro=0$

Bo	Ro	q	za	ra	ψ	β	V2	V1
10.5	0	0.5389	1.0009	1	$\pi/2$	1.0472	3.1446	0.6313
20.5	0	0.2336	0.9633	1	$\pi/2$	1.0472	3.0261	0.5129
30.5	0	0.1145	0.9417	1	$\pi/2$	1.0472	2.9585	0.4453
40.5	0	0.0604	0.9273	1	$\pi/2$	1.0472	2.913	0.3998
50.5	0	0.0338	0.9166	1	$\pi/2$	1.0472	2.8797	0.3663
60.5	0	0.0198	0.9084	1	$\pi/2$	1.0472	2.8537	0.3405
70.5	0	0.0122	0.9018	1	$\pi/2$	1.0472	2.8328	0.3196
80.5	0	0.0079	0.8962	1	$\pi/2$	1.0472	2.8155	0.3022
90.5	0	0.0051	0.8916	1	$\pi/2$	1.0472	2.8008	0.2875

Figure 4.16 is the free surfaces plots for increasing Rotation number with $Bo=25$. The liquid has a contact angle $\alpha = 30^\circ$. Table IX lists the calculated values for each Rotation number.

TABLE IX: Values for Cylinder with $\alpha = 30^\circ$ and $Bo=25$

Bo	Ro	q	za	ra	ψ	β	V2	V1
25	1	0.3085	0.9623	1	$\pi/2$	1.0497	3.0233	0.5114
25	2	0.4484	0.9726	1	$\pi/2$	1.0472	3.0556	0.5424
25	3	0.5874	0.983	1	$\pi/2$	1.0472	3.0882	0.5749
25	4	0.7253	0.9935	1	$\pi/2$	1.0472	3.1213	0.608
25	5	0.8617	1.0042	1	$\pi/2$	1.0472	3.1548	0.6416

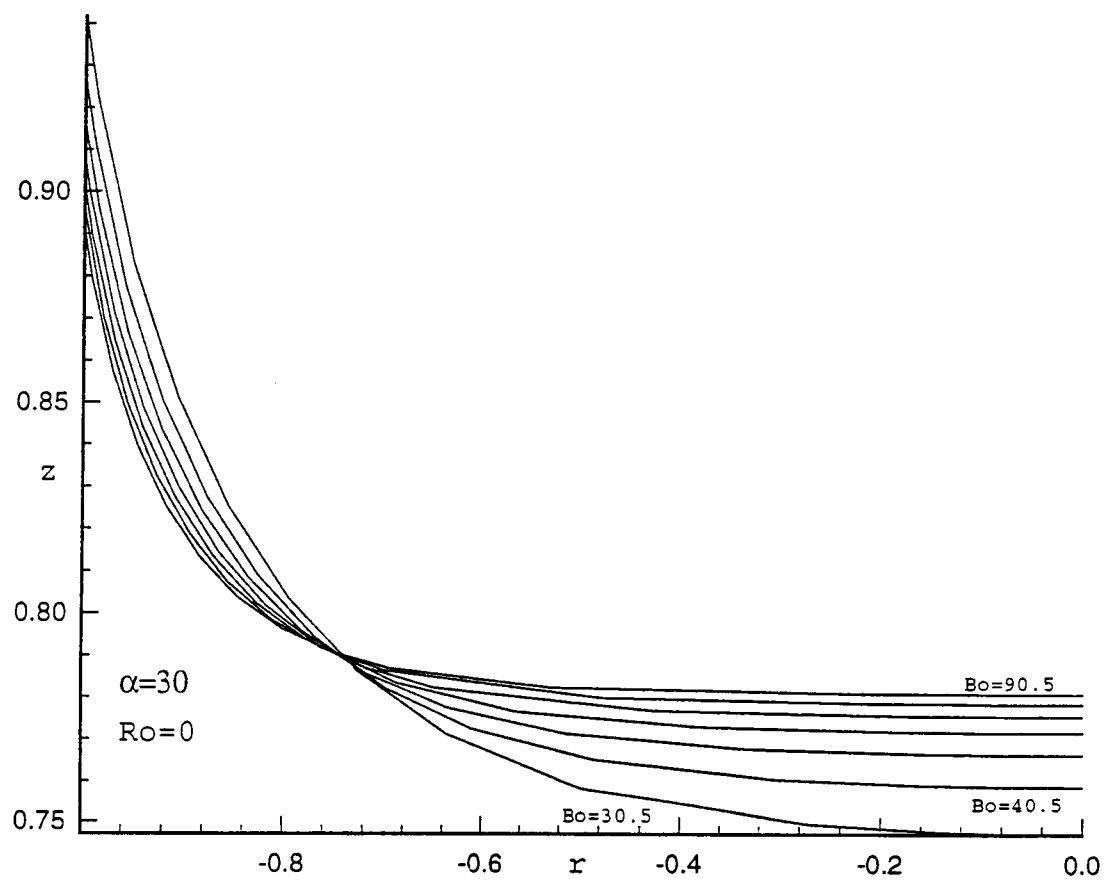


Fig. 4.15: Cylinder with $\alpha=30^\circ$, $Ro=0$, and $Bo=30.5$ to $Bo=90.5$.

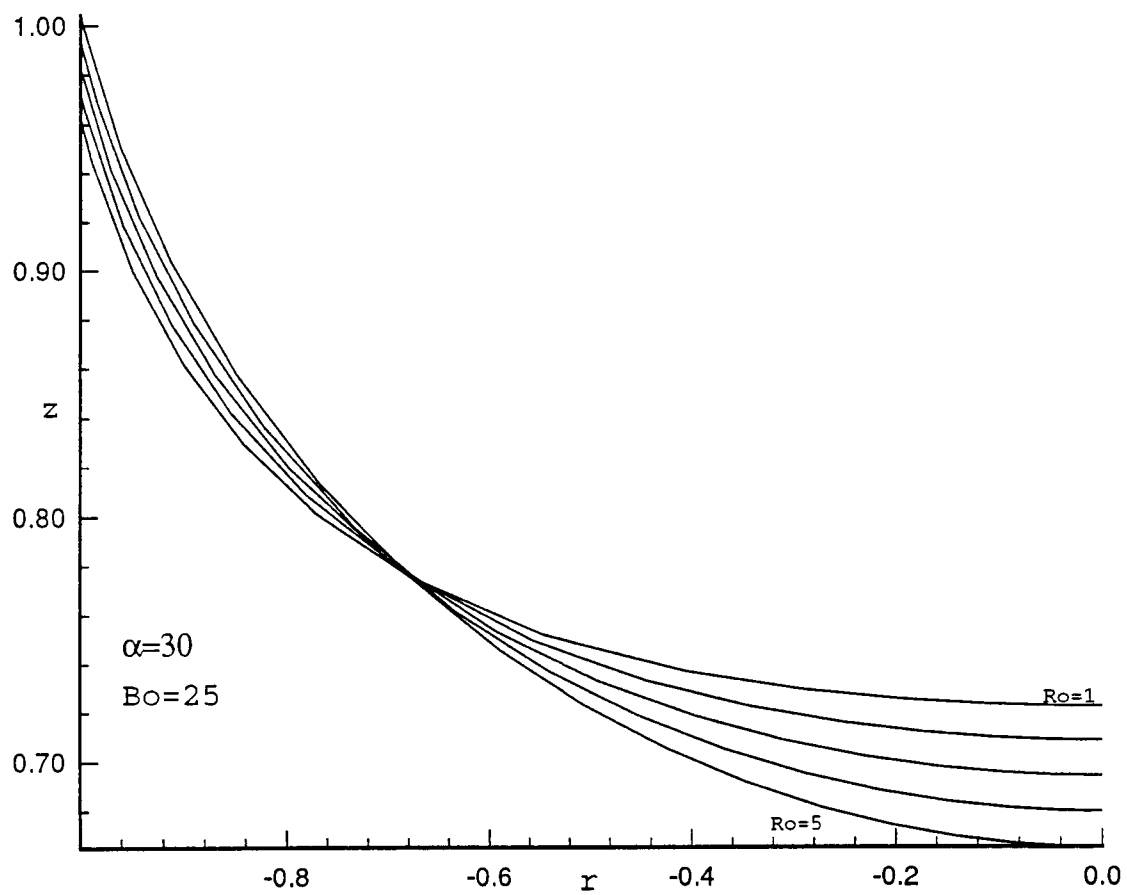


Fig. 4.16: Cylinder with $\alpha = 30^\circ$, $Bo=25$, and $Ro=1$ to $Ro=5$.

4.3 DISCUSSION

There exists some differences between the graphical method and the numerical method which will be discussed next.

Slobozhanin and Tyupstov state in [7] that the section of the ellipsoid that the point (r_A, q_A) exists is determined by analyzing the intersection of the curves $\psi(r) - \alpha$ with $\beta(r, q)$ and $V_2(r) - V$ with $V_1(r)$ at the point (r_A, q_A) .

The problem of determining the position of r_A on the ellipsoid is corrected in the numerical method by changing the functional dependence to z , that is $r = r(z)$, instead of trying to determine z from r . By changing the functional dependence, the problem of determining when r has crossed over the centerline of the ellipsoid is eliminated.

Another difference is a change made to the numerical method after validating it with the example presented in [8]. Both methods were able to obtain two points for the calculation of the free surface, but only one point was physically possible. The elimination the possibility of calculating the nonphysical point was attempted by forcing a reasonable initial value for z .

The initial value for z is found by determining the value of z that will satisfy the following criteria

$$V_2(r(z)) = V \quad (4.3.1)$$

It has been observed that only physically possible free surfaces have been obtained when applying the above criteria, but if the actual value of z is sufficiently far away from the initial starting point then the method is not as successful.

It was observed that the numerical method has difficulties in calculating (z_A, q_A) for large Bond and/or Rotation number(s). The problem arises in choosing an appropriate initial (z_o, q_o) to begin calculations.

The problem is corrected by starting with some base Bond number and Rotation number, Bo_o and Ro_o , and incrementing them by ΔBo and ΔRo until the desired Bo and Ro are reached. As the Bo_o and Ro_o are incremented, the point (z_A, q_A) calculated for the previous Bo and Ro are used as the initial guess in calculating (z_A, q_A) for $Bo_o + \Delta Bo$ or $Ro_o + \Delta Ro$.

If there is rotation for a particular problem, the numerical method handles it by first calculating the free surface for the desired Bo with $Ro=0$. Then Ro is incremented until the desired Ro is reached.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

The numerical method developed in chapter 3 was shown in section 4.1 to produce results comparable to the graphical method by means of the example presented in [7] and is expected to predict more accurate results than the graphical method. Qualitatively, the free surfaces calculated by the numerical method appear to be in agreement with free surfaces obtained by Concus [4] (see Figures 4.2 and 4.3) and the free surfaces shown in [2] (see Figures 4.4, 4.5, 4.6, and 4.7).

From the results presented in section 4.2, the numerical method appears to predict the behavior of the free surface as the pressure distribution p within the fluid is changed either by decreasing or increasing the Bond number and/or the Rotation number. For example, one would expect that as the rotational velocity is increased a depression would form around the axis of symmetry, which can be seen in figures 4.10a,b, 4.12, and 4.14.

Because results of the numerical were only qualitatively compared with other results, the numerical

method should be validated and accuracy checked by experimental data. The method could be compared with experimental data which may already exist or data could be experimentally obtained for microgravity conditions by choosing an appropriate length scale to obtain the desired Bond and Rotation number.

The numerical method needs to be tested on the possible range of fill levels and contact angles to check if there may be any limitations based on those conditions. Also it could be investigated to see if the method can be modified to take into account other physically possible situations, such as change in temperature, change in density, two radii of curvature, etc.

In general, a procedure was developed for calculating the free surface shape of a liquid contained in an axisymmetric vessel under the influence of gravitational and centrifugal forces ,which did not require the memory and speed of a computer workstation, but could be utilized on a 486 based PC system.

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