Drop separation by numerical solution of
the Navier-Stokes equation

by

Dale Alan Fitzgibbons

An Abstract of
A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

Approved:

Lawrence Burkhardt
In Charge of Major Work

MASTER

George Burnett
For the Major Department

M. J. Ulmer
For the Graduate College

Iowa State University
Ames, Iowa

1978

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the Navier-Stokes equation

Dale Alan Fitzgibbons

Under the supervision of Lawrence E. Burkhart
From the Department of Chemical Engineering and Nuclear Engineering
Iowa State University

A numerical model of separating drop behavior was constructed and tested by simulation, on a general purpose digital computer, of a hypothetical two-immiscible-phase system. The model uses the Marker-and-Cell (MAC) method to solve the unsteady state Navier-Stokes (momentum balance) equation with incompressible flow. Input to the model consists of fluid parameters (density, viscosity, interfacial tension), initial conditions (interface profile and velocities), and forcing functions. Simulation results consist of time varying velocity and pressure fields, and all transformations of the interface profile.

The test simulation began with a pendant drop possessing the maximum or critical volume. All fluid elements were initially at rest and all pressures were hydrostatic. The equilibrium was disturbed by application of a gravitation pulse. The profile then deformed as the bulk of the drop accelerated into the surrounding medium. Detachment was successfully achieved, and part of the post-separation behavior was followed. The simulation was seen to exhibit many of the features known to accompany separations observed in the laboratory, including characteristic profiles and flow patterns.

This study had a dual purpose. On one hand it was desired to improve older models designed to predict drop shapes and flow patterns,

combining them into one complete package. On the other hand it was desired to adapt the MAC method, originally developed for very large computers, to average-sized machines with modest memory capacities. Both requirements made it essential to devote considerable attention to developing the boundary condition for the interface. A significant product of this effort is a successful implementation thereof.

The simulation incorporates a one-parameter model of the interface, with the parameter being the equilibrium interfacial tension. Dynamic interfacial tension and interface viscosity are omitted. At each computational time frame the curvature of the interface is computed by numerically fitting a set of cubic splines to the coordinates of the particles which compose the interface. This curvature is used to compute the pressure drop across the phase boundary, and comprises the boundary condition for the calculation of pressures within the drop.

That process requires determination of the second derivatives of the interface curve, and is plagued by numerical errors. These errors, if unchecked, enter into the pressure calculation, thence to the determination of velocities, and ultimately are fed back as more serious errors in the curvature of the interface. This difficulty was overcome by a dual smoothing procedure: the interface was smoothed, then the second derivatives were computed and also smoothed. Well-behaved curvatures were then computed from the smoothed second derivatives.

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CHAPTER 1. INTRODUCTION

The production and movement of fluid drops occupy an important role in many chemical separation processes. In gas absorption, solvent extraction and distillation it is necessary for drops or bubbles of one fluid to form by passage through an orifice, to detach from the orifice, and to travel through the surrounding fluid exchanging mass, momentum, and energy with it. While the design of separation equipment has historically been achieved largely by empirical methods, the need for increasingly efficient equipment and better design tools has fostered considerable interest in learning the nature of fundamental processes. Of primary importance are the formation, separation, transit, and coalescence of drops or bubbles of one fluid within another.

The elemental processes of mass transfer during drop formation (61), transit through a medium (15, 34), and coalescence (6) have been thoroughly investigated. The problem of mass transfer during separation is no less important, but because of the extreme difficulty of observing and measuring this brief event, researchers have largely avoided it. Experimental work in this area usually involves high-speed photographic analysis. The most common procedure is to take motion pictures of forming and separating drops which contain tracer particles (usually aluminum or glass) and measure the motions of the particles from frame to frame. This is not only tedious, but is prone to experimental irreproducibility due to the high sensitivity of surface tension to trace impurities. Furthermore, only internal velocities and profiles

can be studied; internal pressures and solute concentrations are still unavailable.

These considerations make the prospect of constructing a mathematical model of the separation process particularly appealing. Such a model must be accurate, stable, and allow ready observation of velocities, pressures, concentrations, and profiles. The most accurate and complete description of fluid flow phenomena is the set of Navier-Stokes partial differential equations (2) which describes time variations of the rate of momentum transfer in the three spatial directions. These equations, along with the equation of continuity (2) and appropriate boundary conditions, completely and unambiguously describe the flow in a system. The equations, however, are nonlinear and intractable; analytic solutions have been obtained only at the cost of restrictive simplifying assumptions and have required some prior knowledge of the nature of the flow. The advance of large digital computers and special numerical techniques has brought more general solutions to within the realm of reason.

Of the various numerical methods for computing flows, one particularly flexible and powerful one is the Marker and Cell (MAC) method, developed at the Los Alamos Scientific Laboratory (27, 62). Designed to handle incompressible flows, the method uses the full Navier-Stokes equations, facilitates implementation of fixed-surface boundary conditions, and permits direct calculation of internal pressures and velocities. The technique is specifically intended to simulate flows with free surfaces. Unfortunately, free surfaces are by no means easy to manage in any calculation, especially when surface tension is an important factor.

Consequently, each application of the MAC method requires careful analysis and tailoring for the free surface.

To this end, Sandry (52) endeavored to simulate, using the MAC method, the flows and profiles which exist in forming and separating drops of incompressible fluid. To do this he divided the problem into two parts. In one he simulated the flows existing in a suspended stable drop whose volume and profile were held constant by introducing and removing liquid simultaneously through a double concentric nozzle. In the other he began with a static suspended drop in which all material was at rest. The drop was made to become unstable and accelerate toward separation by an abrupt reduction of surface tension. He correctly reasoned that, while each of these regimes only approximated the behavior of an actual separating drop, the actual flow contained elements of each of the approximations.

Sandry's results were significant in that his computed circulation patterns in the forced internal flow calculations agreed very closely with previous experimental results. In addition, his separation profiles resembled experimental profiles well into the separation stage, and certainly past the point at which previous analytical models broke down. Unfortunately, his simulations were never carried to the instance of detachment, but were terminated as the fluid interface began to experience distortions caused by numerical difficulties. It is the express purpose of the present study to correct these distortions and carry the simulation through the point of detachment.

It is worthwhile to review the sequence of events for the separation of a real drop. Figure 1.1 shows the separation of such a drop

Figure 1.1. High-speed photographs of a separating water drop. The sequence was filmed with a Milliken DBM-5C camera at 400 frames per second

of water. The drop is originally hanging from a nozzle and nearly motionless. As fluid enters the drop through the nozzle the volume of the drop increases to a critical value above which the surface tension of the liquid cannot support its weight. The drop begins to elongate, slowly at first, but faster as the bulk of the drop accelerates under the influence of gravity. The region midway between the base and the apex of the drop begins to narrow, both because of the requirement that volume be conserved and due to the driving force of the surface tension. The neck narrows into a thin column of liquid connecting the fluid region at the nozzle (base) to the spheroid region which eventually becomes detached (globe). The phenomenon of Rayleigh-Taylor instability promotes the formation of ripples on the column. These ripples grow in amplitude until they are large enough to cause breakup of the column. In photographic observations of separating drops of various liquids the column always broke first at the globe end of the column, and then almost immediately at the base end. The column then consolidated into a single tiny sphere or became subdivided into smaller droplets. It is being attempted in this study to simulate these events as closely as possible.

CHAPTER 2. REVIEW OF LITERATURE

The theory of the processes governing the formation and separation of liquid drops has become a subject of great concern in recent experimental investigations because of the need for increasingly refined models of mass transfer processes. These systems are extraordinarily complex, and historically have been analyzed only by approximate and empirical means. Early investigations of drop phenomena were largely concerned with determining the effect of various fluid parameters, especially surface tension, on the size of a pendant drop. The object was to improve the accuracy of experimental techniques for measuring the surface tension of a liquid. The accuracy of the so-called drop-weight method (24) depends on the ability to predict the volume of a separated drop.

The emphasis of various studies subsequently shifted to the effect of the shape of a drop on the rate of mass transfer across the interface. While it has long been known that significant mass transfer occurs in a drop freely falling through a continuous liquid or gas phase, it was rather lately observed (12) that a significant portion of the extracted or absorbed solute crossed the phase boundary during the actual formation and separation of the drop. In quest of more detailed knowledge, investigators have more recently attempted to deduce the flow patterns within the drop and to show how they are influenced by fluid parameters.

Correspondingly, the discussion in this chapter is divided into categories pertaining to the sizes of drops, their shapes, and detailed studies of internal velocities and other internal phenomena.

With the advent of high-speed digital computers and the evolution of elegant numerical techniques for solving the equations of flow, it was inevitable that effort would turn to detailed simulations of the behavior of fluid interfaces, and of drops in particular. Consequently, a section is included describing the computational background of this study.

Of course, no clear-cut divisions actually exist in the body of knowledge of drop phenomena; the ones used here are merely arbitrary and convenient. Considerable overlap into other areas is expected of a paper in any category.

Detached Drop Volume

The background for this discussion actually begins with the theoretical investigations of Laplace (39), who derived an equation stating that the pressure difference across a fluid-fluid interface is proportional to the radii of curvature of the interface. Relating this pressure difference to hydrostatic pressures associated with geometry yields an ordinary differential equation describing the shape of the interface curve. The equation is nonlinear and cannot be solved analytically. Bashforth and Adams (1) developed a numerical technique to solve this equation for drop profiles. They solved it for several

cases by laborious hand calculations and reported generalized solutions in tabular form.

Lohnstein (40), in developing the drop-weight method for measuring surface tension made the important observation that growing pendant drops enlarge to a maximum or "critical volume" condition, then become unstable and detach from the main portion of liquid. His method predicts the drop volume using very crude information regarding the shape of the drop at the instant of separation, and his results deviate as much as 30 percent from those of other investigators.

In refining Lohnstein's method, Harkins and Brown (24) discarded his assumption that contact angle is the same before and after separation. They modified Tate's Law (Harkins and Brown, 24) for the weight of an ideal drop by inserting a geometrical correction factor, and wrote

$$w = 2\pi r T \psi (r/v^{1/3}),$$

where w is the actual drop weight, r is the radius at the orifice, T is the surface tension, v is the drop volume, and ψ is a correction factor assumed to be a function only of the profile. Rather than attempting to predict ψ by crude theoretical means, as did Lohnstein, they evolved a simple experimental procedure for calibrating a particular orifice in order to determine the correct value of ψ .

Using variational and numerical methods, Freud and Harkins (14) confirmed Lohnstein's "critical volume" hypothesis. By considering the theoretical profiles of slowly growing hanging drops, they had hoped to develop a precise mathematical relationship between the size

and shape of a hanging drop and the volume of a detached drop. Based on some excellent high-speed (128 frames per second) motion picture studies, they were merely able to establish that the process of detachment was more complex than theretofore imagined. They concluded:

"The theory of the detaching drop has thus been barely touched, and much work must be done upon it before the desired relationship can be found."

Accordingly, many attempts by subsequent investigators to correlate drop volume to measurable quantities either resulted in primitive geometrical models of detaching drops, or produced strictly empirical models.

Hayworth and Treybal (29) used a force balance and dimensional analysis to correlate drop volume to a single free parameter containing all pertinent fluid properties. They were able to predict drop weight with 7.5 percent average error. Rao, Kumar, and Kuloor (51) later refined this with a more elegant force balance and allowed more free parameters. Their average error was 6.8 percent. Poutanen and Johnson (50) fitted experimental profiles of growing bubbles to the empirical model

$$r^n \theta = 1,$$

where r and θ are the usual polar coordinates and n is an adjustable parameter. From this they computed surface area and volume by integration. They did not report their accuracy. Narayanan, Basu, and Roy (45) reported a simple dimensional analysis which gave drop diameters with an accuracy of 10 percent.

Among the less empirical models was that of Null and Johnson (47) who constructed drop profiles from sections of cones, spheres, and cylinders, and correlated them with experimental observations. Manfré (41) used the Hagen-Poiseuille equation and a pressure balance to derive a first-order ordinary differential equation relating the change in drop volume with time. Since he was concerned primarily with the extrusion of glasses and other highly viscous materials, his model works best with flow at very low Reynolds numbers. Scheele and Meister (54) used a force balance to study the effects of orifice diameter and physical properties on drop volume. Their correlation yielded an average 11 percent accuracy. Kumar (36) reported a much more elaborate force balance valid for both bubbles and drops, but which afforded only 15 percent accuracy.

Shape and Volume of Suspended Drops

Work in this area largely parallels the investigations discussed above of means for predicting detached drop volume. Particular emphasis has been given to it more recently as studies of mass transfer processes have proliferated. The articles discussed above are pertinent in varying degrees; later models expressly derived for mass transfer applications will be cited next.

San Giovanni (53) modernized the procedure for integrating Laplace's pressure equation and constructed a digital computer program to perform the required numerical integrations. He was primarily concerned with the effect of the rate of surface area production in a

forming drop on mass transfer across the phase boundary. His model treats growth rate as being infinitesimal, and does not take into account the effect of internal flow on the shape of the drop. All his profiles are mathematically valid static drop profiles, although some of them are physically unlikely.

Halligan and Burkhart (19) showed how dynamic effects could be included in the hydrostatic pressure balance differential equation. They added a linear hydrodynamic pressure term to account for longitudinal motion of fluid along the central axis. Their computed profiles compare favorably with experimental profiles (20) up to the point at which the drop profile develops a radial minimum, i.e., begins "necking in." They concluded that a new model is needed for the interval between developing the minimum and the instant of detachment.

Seemann (57) addressed this problem by considering the effect of internal velocities on the pressure distribution within the neck. Using Bernoulli's equation he derived a correction for the pressure balance used by Halligan and Burkhart (19). This technique produced a model which showed good agreement with experimental profiles in the apex and neck regions of the drop, but failed to predict the base profile correctly.

From this point we take a significant jump in complexity to the numerical simulations of Sandry (52), which were discussed briefly in Chapter 1. Numerical difficulties forced him to use very low values of surface tension (about 6 dynes/cm), and lumps developed in the profile during the advanced stages of separation. He was

never able to achieve actual detachment, but his profiles agreed with experimental profiles well past the point of necking-in.

Internal Flow

In 1950 Dixon and Russell (12) demonstrated that the rate of mass transfer during drop formation is much higher than previously believed. Furthermore, they noted that the mass transfer rate is inversely proportional to the time of formation. They concluded that the turbulence within the drop produced by the jet from the nozzle reduces the resistance to mass diffusion at the interface. However, they did not attempt to predict the flow patterns within forming drops.

Garner and Skelland (16) observed that flow patterns during formation are similar to those existing during the period of free fall after detachment. They found that liquid travels from the nozzle along the central axis to the apex and back along the surface to the base. Increased feed rates give rise to larger mass transfer coefficients by increasing the rate of internal circulation.

Groothuis and Kramers (17) confirmed the findings of Garner and Skelland (16). They also noted that while the rate of absorption is higher for short times of formation, the total quantity of mass transferred is less than for drops formed more slowly. In addition, they found that the rate of transfer appears to decrease as the drop nears detachment due to a possible damping effect of separation. Increased viscosity also dampens circulation, even with high flow rates through the nozzle.

Marsh and Heideger (42) reported a fourteen-fold decrease in mass transfer rate during the first second after formation due to a decay of internal circulation. However, circulation does not disappear completely, but continues after detachment. They showed that the overall amounts of mass transferred in the three phases of a drop's life, formation, one second after formation, and thereafter, are roughly equal.

In an attempt to overcome the difficulty of maintaining and observing internal circulation for an extended period, Constan and Calvert (7) proposed the technique of suspending a drop from two concentric nozzles. Internal circulation is maintained by injecting liquid into the center nozzle and withdrawing an equal amount from the outer annulus. Using this method, Panno and Calvert (49) observed that for two drops of the same size and with the same flow rate, the one with the smaller nozzle experiences greater mass transfer. They concluded that the resulting higher nozzle velocity produces a higher circulation rate.

In their previously-discussed work on drop formation profiles, Halligan and Burkhart (21) also considered internal fluid velocities. They experimentally measured apex velocity and internal fluid velocity by photographing drops containing tracer particles. They characterized internal velocity from the Lagrangian viewpoint by relating it to apex velocity (a measure of the bulk motion of the detaching portion). They found that relative velocity is inversely related to viscosity, and that it is easily fitted to an exponential function.

Weathers (61) further studied circulation in drops with a concentric nozzle and confirmed the damping effect of viscosity. He noted that

sufficient viscosity could eliminate circulation entirely. He also confirmed that with high flow rates or low viscosities circulation could extend well into separation. His high-speed photographs show the types of circulation patterns to be expected for various values of viscosity. Expanding the work of Weathers, Sharer (58) found that the lowest circulation rates produce the lowest mass transfer rates while the highest circulation rates produce the highest mass transfer rates.

In the important numerical study of Sandry (52) discussed above, he also simulated the experiments of Weathers and Sharer. He confirmed the effects of flow rate and viscosity and produced excellent plots of flow patterns.

Numerical Methods

The various methods for solving the fluid flow equations may be placed in three main divisions: analytical, semi-analytical, and numerical. Analytical methods transform the differential equations and boundary conditions into mathematical expressions for the solutions; numerical results are then obtained by evaluating the expressions. These methods invariably require simplifying assumptions which are often too restrictive to allow solutions to realistic problems. Semi-analytical methods generally break the problem into portions to be solved analytically and portions to be solved numerically. Examples are the so-called spectral methods (48) in which velocities are expanded into series of orthogonal functions. Numerical operations are performed

to determine the coefficients of the series. The success of this method depends on the choice of the orthogonal functions, which affects accuracy and solution time. Incorrect selection of the type of series expansion can lead to inefficient and inaccurate simulations.

The most general methods are the numerical or finite-difference schemes, which fall into two broad categories (48): the primitive variable (PV) methods and the vorticity-streamfunction (VS) methods. In the primitive variable methods velocity and pressure are solved directly using finite-difference representations of equations of momentum, continuity, and state. An example of this is the PIC (Particle-in-Cell) method in which mass-bearing particles in cells are used to represent the motion of a "discontinuous fluid." Continuum equations, written in Lagrangian form, are used to compute the movements of the particles. Primitive variable methods are particularly useful in computing low Reynolds number flows.

In the vorticity-streamfunction methods the primitive variables are transformed into the variables vorticity and streamfunction, which are incorporated into modified versions of the flow equations. Whereas pressure in PV methods is effected instantaneously throughout the computation region, vorticity in VS methods is generated at boundaries and diffused and convected into the free stream. Vorticity-streamfunction methods are useful in computing high Reynolds number flows.

The wide range of types of problems in fluid dynamics and the broad array of numerical methods makes it important to be prudent in

one's selection of an approach to a particular application. Emmons (13), Orszag and Israeli (48), and Harlow (25) have provided detailed discussions of the foregoing considerations and present critical overviews of the various numerical techniques, along with the types of problems to which they are best suited.

The approach chosen for this work is the Marker and Cell (MAC) method (27, 62) because of its inherent long-term stability and its ability to manage a moving free surface or interface. The flow region is divided into an array of rectangular or square elements or cells whose sides form the increments of the spatial variables. Superimposed upon this Eulerian mesh is a Lagrangian mesh of particles or markers whose coordinates vary according to local fluid velocities. The purposes of the particles are to follow the motion of the fluid in space and to establish the position of the interface. The technique uses the "motion picture frame" concept in which all cell mesh variables such as pressure and velocity are computed for each cell at one instant, and time is advanced by an increment to the next instant as the particles are moved according to local velocities to their new positions. The procedure uses an error correction scheme which allows roundoff and truncation errors developing in one time frame to be removed in the next time frame. Residual errors from many time steps are thus prevented from accumulating, and excellent long-term stability is possible. This "elimination of residual error" concept has been generalized for application to any arbitrary initial value problem (31).

While the MAC method is well-suited to handling a large number of configurations it is best known for its ability to implement a

free surface or interface. In early applications of the method the free surface was simply the boundary between the region of cells containing particles and the region of empty cells; no special consideration was given to this boundary. To facilitate computation of particle motions at the free surface the requirement was made that the first derivatives of the coordinate components of velocity be zero in this region. A number of computational examples are given in the original reports (27, 62).

Although the approach facilitates the modelling of a free surface, such a surface never has been easy to simulate, even for the MAC method. Consequently, considerable work has since been devoted to this problem. Daly (8) investigated the occurrence of Rayleigh-Taylor instability at the interface between two immiscible liquids. In this early study the interface was resolved only to one cell width, and no special attention was given to boundary stress conditions at the interface. Later Daly (9) evolved a means of adding surface tension to this type of calculation. A special set of particles would be designated to mark the boundary between the two phases. A set of cubic splines would be used to interpolate values between the particle positions, and local surface tension pressure would be calculated from the curvature of the interface sequence using Laplace's pressure balance. The computed surface tension pressure would then be applied directly to the nearest cell center. With this new tool, Daly (10) enlarged his earlier study (8) to include surface tension effects. He found that surface tension particularly enhances the growth of physical instabilities, and presented good plots of "spike" breakup at an unstable interface.

Hirt and Shannon (32) presented the rigorous normal and tangential stress boundary conditions for the free surface. They developed a simple and convenient approximation to the normal stress condition and showed how it could improve the accuracy of low Reynolds number calculations. Their method omitted normal stress due to surface tension. Chan and Street (5) subsequently pointed out that difficulties may arise when an external pressure is applied not at the true surface but at a nearby cell center. They modified the finite difference formulas containing pressure to allow uneven spacing for the pressure contribution of an arbitrarily-positioned free surface. Nichols and Hirt (46) combined the method of Chan and Street with the simple free surface normal and tangential stress conditions suggested by Hirt and Shannon to obtain a more complete and reliable approach.

In a related vein, Vieceilli (59) suggested a means of including arbitrary curved fixed boundaries in a MAC calculation. This scheme adds a corrective pressure term which forces liquid to flow tangentially to a curved fixed boundary. Vieceilli (60) later expanded this technique to enable the use of moving boundaries.

Other examples of the use of the MAC method are by Daly and Pracht (11), who studied density-current surges, and by Harlow and Shannon (28) who investigated the splash and coalescence of a liquid drop on a solid surface, a deep pool, and a shallow pool.

Of primary importance is the stability of the simulation. Since the equations of motion are nonlinear, classical stability theory fails here. Hirt (30) addressed this problem by expanding the finite difference equations used in the MAC method into Taylor series. The

first-order terms form linear differential equations which are subjected to a rigorous stability analysis; higher-order terms are dismissed as truncation errors.

CHAPTER 3. THEORY

General Remarks

In order to simulate the behavior of separating liquid drops it is necessary to construct a mathematical description of the phenomenon. Before this can be done specific statements about the nature of the flows must be made, and the scope of analysis must be established.

In this regard it should be understood that all flows in this study are incompressible and Newtonian. Furthermore, homogeneous phases possess constant and uniform density, and heat effects are assumed negligible.

Fluid dynamics problems may be viewed as consisting of three parts: (1) input data, containing all knowledge of fluid properties, initial conditions, boundary conditions, and forcing functions; (2) the system, containing mathematical statements relating dynamical causes with effects; and (3) output data, consisting of all consequent fluid motions. "Solving the problem" consists of applying by suitable means the input data to the system in order to produce the desired output data. Typically, the mathematical statements composing the system are in the form of differential equations relating the changes in momentum of a volume element of fluid to forces applied from outside the element.

Many simple problems are easily solved by constructing a "shell momentum balance" in which the volume element is an annulus or an infinite sheet of infinitesimal width. An example of this type of analysis is the derivation of the well-known Hagen-Poiseuille equation (2, p. 46) for laminar flow in a cylindrical tube. Because of its

limited compass, this method usually can be applied only to one-dimensional and the simplest two-dimensional problems.

Occasionally, a problem is amenable to solution by use of a property peculiar to the particular flow system being considered. For example, much can be learned of the macroscopic nature of flow in a duct by use of the mechanical energy balance of Bernoulli (2, p. 212). The scope of such an analysis will usually not yield detailed information about the flow and, in some circumstances, may prove completely inadequate. The failure of the models of Halligan and Burkhart (19) and of Seemann (57) may be cited as examples. Each of these was intended to predict profiles of separating drops, each was a simplified one-dimensional analysis, and each became inadequate under circumstances emphasizing the multidimensional character of the flow.

The only completely general, universally applicable description of the dynamical behavior of a fluid is the Navier-Stokes equation (2, p. 76) which predicts the changes in momentum in three dimensions and in time for an arbitrary volume element. When supplied with the equation of continuity, an equation of state, and appropriate initial and boundary conditions, the Navier-Stokes equation constitutes a completely adequate description of a flow system. Analysts generally recommend starting with the completely general continuum equations (Navier-Stokes, continuity, and state) followed by elimination of unnecessary terms; this process minimizes the chance of inadvertently omitting important terms, as is possible when using shell momentum balances.

Although rigorous closed-form solutions of the Navier-Stokes equation usually cannot be obtained, a great many useful solutions can be had by analytically solving simplifications of the equation for specific situations. For example, elimination of one or more spatial coordinates will often yield time-variant differential equations which may readily be integrated. Removal of the time derivative will produce steady state solutions. An important class of solutions are reached by assuming "ideal flow" which uses constant density and zero viscosity. At the opposite end of the spectrum are the "boundary layer" solutions in which viscous effects predominate. Ideal flow solutions are sometimes combined with boundary layer solutions to describe completely the flow in a system.

Correspondingly, the full Navier-Stokes equation is used in this study to describe all flows. Due to the geometrical complexity of the flow regions used very few simplifications can be made. The ideal flow and boundary layer models are eliminated outright. The transient nature of the problem requires retention of time derivatives of velocity. Proper choice of the coordinate system and the use of symmetry will permit elimination of one spatial coordinate. Assumption of constant density entails use of a trivial equation of state. No major term in the Navier-Stokes equation is categorically removed. The equation, in essentially uncut form, cannot be solved analytically. Consequently,

all equations are recast as finite difference equations¹ and the set is solved numerically.

As discussed in the last chapter a number of finite difference techniques have been proposed for solving the full Navier-Stokes equation. The difficulties cited with the spectral methods (48) cause them to be dismissed outright from serious contention. Furthermore, vorticity-streamfunction methods make it awkward to apply a workable free surface or interface boundary condition. Hirt, Cook, and Butler (33) categorically reject vorticity-streamfunction methods for such applications. Elimination of these two categories leaves only the primitive variable methods as contenders.

A list of the requirements which must be met by a primitive variable technique may be established. The technique must:

1. Allow observation of bulk fluid motion;
2. Facilitate implementation of a free surface boundary condition with surface tension;
3. Facilitate implementation of boundary conditions at walls and lines of symmetry;
4. Possess built-in momentum and volume conservation;
5. Maintain long-term accuracy and stability;
6. Enable representation of multiple fluids.

A review of available methods produces several likely candidates. The

¹One might argue that this alone constitutes a simplification. The matter is largely philosophical; the author feels that the finite difference approximations are merely an algebraic gimmick, do not fundamentally alter the way in which the flow is described, and do not fit the implied definition of "simplification" as used in the previous paragraph.

most noteworthy are the CEL (13), the PIC (13), the MAC (62), and the ICE (26) methods.

The CEL (Combined Eulerian-Lagrangian) method is well-suited to fluid dynamics problems involving moving phase discontinuities such as solid objects driven by shock waves. Eulerian forms of the finite difference equations are used to describe the motion of the bulk of fluid, while Lagrangian representations are used at the surfaces.

The PIC (Particle-in-Cell) method uses a Eulerian mesh of stationary cells used to express finite difference forms of the continuum equations. The fluid is represented by a set of particles or mass points distributed among the cells according to local fluid density. The motion of the fluid is easily observed and mass conservation is guaranteed. Continuity is not maintained because the fluid consists of mass points and is not continuous.

The MAC (Marker-and-Cell) method superficially resembles the PIC method in that it, too, uses particles to represent the fluid and cells to frame the continuum equations. In this case, however, the particles do not represent mass, and conservation of mass, momentum and volume are maintained by careful handling of the continuum equations. The MAC method is expressly designed to permit observation of fluid motion, especially with a free surface or interface. A version is also available to handle multiple immiscible fluids in contact with each other. Recent modifications facilitate application of free surface stress boundary conditions (32), surface tension (9), and curved boundaries (59). Boundary conditions at walls and lines of symmetry are easily implemented, and the method uses a negative feedback

technique to prevent residual error from accumulating in time.

The ICE (Implicit Continuous-Fluid Eulerian) method is actually an extension of the MAC method and has been successful in computing flows in all velocity ranges, including supersonic. In the incompressible limit the technique reduces to the MAC method.

Comparison of these methods shows that the MAC method is undoubtedly the best choice for use in this study. This is reinforced by the fact that it has been used by Daly (10) to study unstable liquid interfaces with surface tension. In that work several drop-like shapes were simulated.

The Continuum Equations

The solution of any problem of fluid dynamics, regardless of the technique used or manner of representing variables, entails the determination of five quantities at all points in the region and for all time. These are three coordinate components of fluid velocity, pressure, and density. As many equations must be included in the construction of the solution as there are variables. The Navier-Stokes equation, a momentum balance, provides three equations. The continuity equation, a fluid mass balance, provides a fourth, and a state equation, relating fluid density to pressure, temperature, and solute concentration, provides a fifth. A thermal energy balance and a solute mass balance may furnish temperature and solute concentration, if needed. Since this study does not directly concern heat or mass transfer, the last two equations will not be considered.

The continuity equation is derived in general form by Bird, Stewart, and Lightfoot (2) and is

$$\frac{D\rho}{Dt} = -\rho(\bar{\nabla} \cdot \bar{U}) \quad (3.1)$$

where ρ is local fluid density and $\bar{U}$ is the local velocity vector. Equation (3.1) expresses density changes, seen by an observer moving with the fluid, as being proportional to the divergence of velocity.

The Navier-Stokes equation is also presented by Bird, Stewart, and Lightfoot (2); its general form is

$$\rho \frac{D\bar{U}}{Dt} = -\bar{\nabla}p - \bar{\nabla} \cdot \bar{\tau} + \rho\bar{g} \quad (3.2)$$

in which p is local pressure, $\bar{\tau}$ is the stress tensor, and $\bar{g}$ is the gravity vector. Equation (3.2) expresses fluid accelerations seen by an observer moving with the fluid and caused by spatial pressure differences, deformation of the fluid, and gravitational force.

The state equation follows directly from the incompressibility requirement, which is

$$\bar{\nabla} \cdot \bar{U} = 0 \quad (3.3)$$

In the absence of heat and concentration effects, this entails the trivial condition

$$\rho = \text{constant} \quad (3.4)$$

in each homogeneous phase. It should be emphasized that Equation (3.4) is merely a consequence of the more rigorous Equation (3.3). This construction permits the solution technique, to be described subsequently,

to handle more general problems involving heat and mass transfer, and compressibility.

The momentum Equation (3.2) is not in a form suitable for numerical solution, but may be transformed by appropriate manipulations. The substantial derivative on the left side may be expanded using the definition

$$\rho \frac{D\bar{U}}{Dt} = \rho \frac{\partial \bar{U}}{\partial t} + \rho (\bar{U} \cdot \bar{\nabla}) \bar{U} \quad (3.5)$$

Combining this with Equation (3.1),

$$\rho \frac{D\bar{U}}{Dt} = \rho \frac{\partial \bar{U}}{\partial t} + \rho (\bar{U} \cdot \bar{\nabla}) \bar{U} + \bar{U} \left[\frac{D\rho}{Dt} + \rho (\bar{\nabla} \cdot \bar{U}) \right]$$

or

$$\rho \frac{D\bar{U}}{Dt} = \rho \frac{\partial \bar{U}}{\partial t} + \rho (\bar{U} \cdot \bar{\nabla}) \bar{U} + \bar{U} \left[\frac{\partial \rho}{\partial t} + (\bar{\nabla} \rho) \cdot \bar{U} + \rho (\bar{\nabla} \cdot \bar{U}) \right]$$

Combining the second and third terms in brackets and rearranging,

$$\rho \frac{D\bar{U}}{Dt} = \rho \frac{\partial \bar{U}}{\partial t} + \bar{U} \frac{\partial \rho}{\partial t} + \rho (\bar{U} \cdot \bar{\nabla}) \bar{U} + \bar{U} [\bar{\nabla} \cdot (\rho \bar{U})]$$

Using formulas for differentiation of products this may be condensed into

$$\rho \frac{D\bar{U}}{Dt} = \frac{\partial (\rho \bar{U})}{\partial t} + \bar{\nabla} \cdot (\rho \bar{U} \bar{U}) \quad (3.6)$$

The viscous diffusion term in Equation (3.2) must be modified to relate it to flow parameters and variables. Brodkey (3) develops an analytical expression of the stress tensor for a Newtonian fluid, leaving it in the form

$$\bar{\tau} = -\mu[\bar{\nabla}\bar{U} + \widetilde{\bar{\nabla}\bar{U}}] + \left(\frac{2}{3}\mu - \kappa\right)(\bar{\nabla} \cdot \bar{U})\bar{I} \quad (3.7)$$

in which μ is the fluid viscosity, κ is the bulk viscosity, $\bar{I}$ is the unit tensor or idemfactor, and $\widetilde{\bar{\nabla}\bar{U}}$ is the transpose of the dyad $\bar{\nabla}\bar{U}$.

The stress tensor is symmetric. Forming the divergence of both sides of Equation (3.7),

$$\begin{aligned} -\bar{\nabla} \cdot \bar{\tau} &= \bar{\nabla} \cdot [\mu\bar{\nabla}\bar{U} + \mu\widetilde{\bar{\nabla}\bar{U}}] - \bar{\nabla} \cdot \left[\left(\frac{2}{3}\mu - \kappa\right)(\bar{\nabla} \cdot \bar{U})\bar{I}\right] \\ &= \bar{\nabla} \cdot [(\mu\bar{\nabla})\bar{U}] + \bar{\nabla} \cdot (\mu\widetilde{\bar{\nabla}\bar{U}}) - \bar{\nabla} \cdot \left[\left(\frac{2}{3}\mu - \kappa\right)(\bar{\nabla} \cdot \bar{U})\bar{I}\right] \end{aligned}$$

using the identities

$$\bar{\nabla} \cdot [(a\bar{\nabla})\bar{A}] = (\bar{\nabla} \cdot a\bar{\nabla})\bar{A}$$

$$\bar{\nabla} \cdot (\widetilde{a\bar{\nabla}})\bar{A} = (\bar{\nabla} \cdot a\bar{\nabla})\bar{A} + \bar{\nabla} \times (a\bar{\nabla} \times \bar{A})$$

$$\bar{\nabla} \cdot (a\bar{T}) = a(\bar{\nabla} \cdot \bar{T}) + (\bar{\nabla}A) \cdot \bar{T}$$

on the first, second, and third terms respectively,

$$-\bar{\nabla} \cdot \bar{\tau} = (\bar{\nabla} \cdot \mu\bar{\nabla})\bar{U} + (\bar{\nabla} \cdot \mu\bar{\nabla})\bar{U} + \bar{\nabla} \times (\mu\bar{\nabla} \times \bar{U}) - \bar{\nabla} \cdot \left[\left(\frac{2}{3}\mu - \kappa\right)(\bar{\nabla} \cdot \bar{U})\bar{I}\right]$$

or

$$-\bar{\nabla} \cdot \bar{\tau} = 2(\bar{\nabla} \cdot \mu\bar{\nabla})\bar{U} + \bar{\nabla} \times (\mu\bar{\nabla} \times \bar{U}) - \bar{\nabla} \cdot \left[\left(\frac{2}{3}\mu - \kappa\right)(\bar{\nabla} \cdot \bar{U})\bar{I}\right] \quad (3.8)$$

Combining Equations (3.6) and (3.8) with Equation (3.2) gives a more useful form of the momentum equation,

$$\begin{aligned}
\frac{\partial(\rho \bar{u})}{\partial t} &= - \bar{\nabla} \cdot (\rho \bar{u} \bar{u}) - \bar{\nabla} p + 2(\bar{\nabla} \cdot \mu \bar{\nabla}) \bar{u} + \bar{\nabla} \times (\mu \bar{\nabla} \times \bar{u}) \\
&= \bar{\nabla} \left[\left(\frac{2}{3} \mu - \kappa \right) (\bar{\nabla} \cdot \bar{u}) \right] + \rho \bar{g}
\end{aligned} \tag{3.9}$$

Equation (3.9) also maintains rigorous momentum conservation, a property held to be valuable by some proponents of finite difference methods (62). This may be demonstrated by integration Equation (3.9) over an arbitrary volume V giving

$$\begin{aligned}
\int_V \frac{\partial(\rho \bar{u})}{\partial t} dV &= - \int_V \bar{\nabla} \cdot (\rho \bar{u} \bar{u}) dV - \int_V \bar{\nabla} p dV \\
&\quad + 2 \int_V (\bar{\nabla} \cdot \mu \bar{\nabla}) \bar{u} dV + \int_V \bar{\nabla} \times (\mu \bar{\nabla} \times \bar{u}) dV \\
&\quad - \int_V \bar{\nabla} \left[\left(\frac{2}{3} \mu - \kappa \right) (\bar{\nabla} \cdot \bar{u}) \right] dV + \int_V \rho \bar{g} dV
\end{aligned}$$

Using the Gauss Divergence Theorem, Leibnitz' Rule, and the identity

$$\int_V (\bar{\nabla} \times \bar{A}) dV = \int_S (\bar{n} \times \bar{A}) dS \text{ (which can be derived from the Divergence Theorem),}$$

$$\begin{aligned}
\frac{\partial}{\partial t} \int_V \rho \bar{u} dV &= - \int_S (\bar{n} \cdot \bar{u}) \rho \bar{u} dS - \int_S \bar{n} p dS \\
&\quad + 2 \int_S \bar{n} \cdot (\mu \bar{\nabla} \bar{u}) dS + \int_S \bar{n} \times (\mu \bar{\nabla} \times \bar{u}) dS \\
&\quad + \int_S \bar{n} \left[\left(\frac{2}{3} \mu - \kappa \right) (\bar{\nabla} \cdot \bar{u}) \right] dV + g \int_V \rho dV
\end{aligned} \tag{3.10}$$

Here S is the surface bounding V and $\bar{n}$ is the unit outer normal vector at S . Equation (3.10) shows that the changes in momentum in V are due only to fluxes across S and to body forces. The form of the momentum

convection term in Equation (3.2) would not have admitted transformation to a surface integral. Finite difference representations of the modified form will approach rigorous conservation as well as the finite difference approximation will permit. Specifying incompressibility, i.e. combining Equation (3.9) with Equation (3.3), eliminates a viscous term, leaving

$$\frac{\partial(\rho\bar{U})}{\partial t} = -\bar{\nabla} \cdot (\rho\bar{U}\bar{U}) - \bar{\nabla}p + [2(\bar{\nabla} \cdot \mu\bar{\nabla})\bar{U} + \bar{\nabla} \times (\mu\bar{\nabla} \times \bar{U})] + \rho\bar{g} \quad (3.11)$$

Although it is anticipated that homogeneous fluid phases will possess constant density and viscosity, Equation (3.11) is the form of the momentum equation required by the multiple-fluid MAC method to account for momentum changes at the fluid interface caused by differences in properties of the contacting fluids. Equation (3.11) is also the starting point for simulations of incompressible flows induced by density gradients (11) such as those existing in heat transfer and mass transfer situations.

It may be noted that pressure appears implicitly in Equation (3.11), while the time derivatives of velocity are explicit. In the exposition of the solution technique it will become apparent that some explicit equation for computing pressures from velocities is highly desirable. Such an equation may easily be derived by forming the divergence of Equation (3.11). This is

$$\begin{aligned} \bar{\nabla} \cdot \frac{\partial(\rho\bar{U})}{\partial t} = & -\bar{\nabla} \cdot [\bar{\nabla} \cdot (\rho\bar{U}\bar{U})] - \bar{\nabla} \cdot (\bar{\nabla}p) \\ & + \bar{\nabla} \cdot [2(\bar{\nabla} \cdot \mu\bar{\nabla})\bar{U} + \bar{\nabla} \times (\mu\bar{\nabla} \times \bar{U})] + \bar{\nabla} \cdot (\rho\bar{g}) \end{aligned}$$

or

$$\begin{aligned} \frac{\partial}{\partial t} [\bar{\nabla} \cdot (\rho \bar{U})] = & - \bar{\nabla} \cdot [\bar{\nabla} \cdot (\rho \bar{U} \bar{U})] - \nabla^2 p \\ & + 2 \bar{\nabla} \cdot [(\bar{\nabla} \cdot \mu \bar{\nabla}) \bar{U}] + \bar{\nabla} \cdot [\bar{\nabla} \times (\mu \bar{\nabla} \times \bar{U})] + (\bar{\nabla} \cdot \rho) \bar{g} \end{aligned}$$

Using the identities

$$(\bar{\nabla} \cdot a \bar{\nabla}) \bar{A} = a \nabla^2 \bar{A} + (\bar{\nabla} a \cdot \bar{\nabla}) \bar{A}$$

$$\nabla^2 \bar{A} = \bar{\nabla} (\bar{\nabla} \cdot \bar{A}) - \bar{\nabla} \times (\bar{\nabla} \times \bar{A})$$

$$\bar{\nabla} \times (a \bar{\nabla} \times \bar{A}) = a [\bar{\nabla} \times (\bar{\nabla} \times \bar{A})] + \bar{\nabla} a \times (\bar{\nabla} \times \bar{A})$$

$$\bar{\nabla} \cdot (\bar{A} \times \bar{B}) = \bar{B} \cdot (\bar{\nabla} \times \bar{A}) - \bar{A} \cdot (\bar{\nabla} \times \bar{B})$$

this becomes

$$\begin{aligned} \frac{\partial}{\partial t} [\bar{\nabla} \cdot (\rho \bar{U})] = & - \bar{\nabla} \cdot [\bar{\nabla} \cdot (\rho \bar{U} \bar{U})] - \nabla^2 p \\ & + 2 \bar{\nabla} \cdot [\mu \bar{\nabla} (\bar{\nabla} \cdot \bar{U})] - \mu \bar{\nabla} \cdot [\bar{\nabla} \times (\bar{\nabla} \times \bar{U})] + 2 \bar{\nabla} \cdot (\bar{\nabla} \mu \cdot \bar{\nabla}) \bar{U} \\ & + \bar{\nabla} \cdot [\bar{\nabla} \mu \times (\bar{\nabla} \times \bar{U})] + (\bar{\nabla} \cdot \rho) \bar{g} \end{aligned}$$

Since $\bar{\nabla} \cdot \bar{U} = 0$ and $\bar{\nabla} \cdot (\bar{\nabla} \times \bar{U}) = 0$, this may be written

$$\begin{aligned} \nabla^2 p = & - \bar{\nabla} \cdot [\bar{\nabla} \cdot (\rho \bar{U} \bar{U})] - \frac{\partial}{\partial t} [\bar{\nabla} \cdot (\rho \bar{U})] \\ & + 2 \bar{\nabla} \cdot (\bar{\nabla} \mu \cdot \bar{\nabla}) \bar{U} + \bar{\nabla} \cdot [\bar{\nabla} \mu \times (\bar{\nabla} \times \bar{U})] + (\bar{\nabla} \cdot \rho) \bar{g} \quad (3.12) \end{aligned}$$

Equation (3.12) may, in principle, be solved to obtain the pressure field for any set of velocity, density, and viscosity fields.

However the assumption that density and viscosity are constant in

each phase may be used to achieve an important simplification. In that case, Equation (3.12) becomes

$$\nabla^2 p = - \rho_\phi \left(Q + \frac{\partial D}{\partial t} \right) \quad (3.13)$$

in which

$$Q = \bar{\nabla} \cdot [\bar{\nabla} \cdot (\bar{u}\bar{u})]$$

$$D = \bar{\nabla} \cdot \bar{u}$$

and ρ_ϕ is the uniform density of the fluid phase. As will be demonstrated subsequently, there is considerable advantage to be gained by solving Equation (3.13) in each phase, rather than attempting to integrate Equation (3.12) across the discontinuity formed by the phase boundary.

It should be noted that the divergence of velocity is left in the time derivative of Equation (3.13), rather than set identically to zero, as has been done previously. Special handling of this derivative is the essential feature of the MAC method which gives it the ability to maintain high accuracy and stability over the duration of long-running simulations.

Description of the Drop Flow Problem

With the establishment of the general mathematical framework necessary for the simulation of incompressible multiple-phase flow situations the details of the drop flow problem may be set forth. Figure 3.1 depicts a typical pendant or suspended drop, showing the two fluid phases, nozzle, apex, contact point, and coordinate system.

Figure 3.1. A pendant (suspended) drop, showing the drop profile, continuous and discontinuous phases, and the coordinate system

Because typical drops tend to be essentially axisymmetric cylindrical coordinates were chosen with the origin near the base of the drop. In this study the drop and all flows therein are assumed symmetric with respect to the z -axis. Therefore only half is shown in the figure, and only half is used in the calculations. Furthermore this symmetry permits all azimuthal variations to be eliminated outright; θ components of velocity and all derivatives with respect to θ are identically zero. This eliminates one differential equation from the formulation, and entails considerable simplification of the others.

The expansion of the momentum Equation (3.11) in cylindrical coordinates is lengthy, and has been placed in the Appendix. The r and z components are

$$\begin{aligned} \frac{\partial(\rho u)}{\partial t} = & -\frac{1}{r} \frac{\partial(\rho r u^2)}{\partial r} - \frac{\partial(\rho u v)}{\partial z} - \frac{\partial p}{\partial r} + 2 \frac{\partial}{\partial r} \left(\mu \frac{\partial u}{\partial r} \right) \\ & + 2\mu \frac{\partial}{\partial r} \left(\frac{u}{r} \right) + \frac{\partial}{\partial z} \left[\mu \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} \right) \right] + \rho g_r \end{aligned} \quad (3.14)$$

$$\begin{aligned} \frac{\partial(\rho v)}{\partial t} = & -\frac{1}{r} \frac{\partial(\rho r u v)}{\partial r} - \frac{\partial(\rho v^2)}{\partial z} - \frac{\partial p}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} \right) \right] \\ & + 2 \frac{\partial}{\partial z} \left(\mu \frac{\partial v}{\partial z} \right) + \rho g_z \end{aligned} \quad (3.15)$$

In which u and v are the r and z components of velocity. In addition, the divergence is

$$D = \bar{\nabla} \cdot \bar{U} = \frac{1}{r} \frac{\partial(r u)}{\partial r} + \frac{\partial v}{\partial z} \quad (3.16)$$

and the requirement $D = 0$ for incompressibility is made. Equations (3.14)-(3.16) are the ones used by Daly (10) in his computational study of unstable liquid interfaces. In the present study the r component of

gravity is eliminated and, with only a moderate loss of generality, the viscosities of both phases are set equal. Equations (3.14) and (3.15) become

$$\frac{\partial(\rho u)}{\partial t} = -\frac{1}{r} \frac{\partial(\rho r u^2)}{\partial r} - \frac{\partial(\rho u v)}{\partial z} - \frac{\partial p}{\partial r} + \mu \frac{\partial}{\partial z} \left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r} \right) \quad (3.17)$$

$$\frac{\partial(\rho v)}{\partial t} = -\frac{1}{r} \frac{\partial(\rho r u v)}{\partial r} - \frac{\partial(\rho v^2)}{\partial z} - \frac{\partial p}{\partial z} - \frac{\mu}{r} \frac{\partial}{\partial r} \left[r \left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r} \right) \right] + \rho g \quad (3.18)$$

The pressure Equation (3.13) in expanded form is

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial p}{\partial r} \right) + \frac{\partial^2 p}{\partial z^2} = -\rho_\phi \left(Q + \frac{\partial D}{\partial t} \right) \quad (3.19)$$

where

$$Q = \frac{1}{r} \frac{\partial^2 (r u^2)}{\partial r^2} + \frac{2}{r} \frac{\partial^2 (r u v)}{\partial r \partial z} + \frac{\partial^2 (v^2)}{\partial z^2} \quad (3.20)$$

Equations (3.14), (3.15) or (3.17), (3.18) and (3.16), (3.19), (3.20), along with appropriate initial and boundary conditions, provide the mathematical framework needed to solve a number of incompressible axisymmetric flows, including single or multiple phase flow in circular or annular ducts, around obstacles, or flows considerably removed from any solid barrier. They may be used to simulate any period in the life of a drop travelling in a medium, from its growth and detachment at a nozzle, through its transit, to its ultimate coalescence. The present study focuses on the detachment phase, starting with a critically stable hanging drop. The solution begins with a hydrostatic situation, i.e., a drop in mechanical equilibrium. All fluid elements are initially at rest, and all pressures are established hydrostatically by elevation. The equilibrium is disturbed by suitable means, and the resulting imbalance

of forces causes fluid elements to be accelerated under the governance of the momentum equations and the continuity equation.

In an unsteady state flow of this type more is needed than simply velocity and pressure information as they change with time. Required is an accurate means of keeping track of the displacements of fluid elements, and of the overall deformation of the fluids. Although the MAC method provides the means for observing displacements and deformations these alone are inadequate for this study. The position and shape of the interface itself must also be included in the prescription of the free surface boundary condition. This fact makes such a free surface flow situation unique among hydrodynamics problems. Ordinarily, while boundary conditions determine the nature of the flow, they are independent of the flow itself. In this problem, however, flow and boundary conditions together form a feedback loop. This fact places supreme importance on careful formulation of the free surface boundary condition.

Initial Conditions and Boundary Conditions

Specifications of initial conditions for transient flow problems can be as varied as the problems themselves. A typical specification, and the one used in this work, is that all fluid be initially at rest. The initial condition for velocity is therefore

$$\bar{U} = 0 \quad (3.21)$$

The initial condition for pressure is easily derived by applying

Equation (3.21) to the momentum equation. Consequent elimination of all velocity-dependent terms leaves only

$$\bar{\nabla}p = \bar{\rho}g \quad (3.22)$$

The details of applying Equation (3.22) to a drop flow problem are provided in the next chapter.

Boundary conditions for velocity and pressure must be specified for all time. They are of two types: those which provide relationships at fixed boundaries or lines of symmetry, and those which provide relationships at free surfaces or interfaces.

The fixed surface boundary conditions are readily derived for walls and lines of symmetry which coincide with coordinate surfaces. The normal component of velocity must always vanish. To reproduce the no-slip behavior one observes in actual flows the tangential component of velocity should also vanish.

However, forcing the tangential component to zero in finite difference simulations can give solutions the appearance of excessive drag at the boundary. The reason for this is that the limited resolution of the finite difference approximation may be insufficient to allow accurate representation of the boundary layer. This problem may be overcome by forcing the normal derivative of velocity, rather than the velocity itself, to zero (free-slip). The question is essentially one of scale. A large fluid region, in which the boundary layer is negligibly thin by comparison, may be adequately modelled using the free-slip requirement, while a smaller fluid region with an appreciably

large boundary layer may require the no-slip requirement. A line of symmetry should always use the free-slip condition.

Accordingly, the boundary conditions for velocity are

$$U_n = 0 \quad (3.23)$$

$$U_t = 0 \text{ or } \frac{\partial U_t}{\partial x_n} = 0 \quad (3.24)$$

in which the subscripts n and t denote normal and tangential components. Normal derivatives of pressure must also be defined for the free-slip and no-slip cases such that they fit the momentum equations. They are derived by substituting the velocity derivatives into the momentum equations, and take the form

$$\frac{\partial p}{\partial x_n} = \rho g_n \quad (3.25)$$

for the free-slip situation and

$$\frac{\partial p}{\partial x_n} = f\left(\frac{\partial U_n}{\partial x_n}, \frac{\partial^2 U_n}{\partial x_n^2}\right) + \rho g_n \quad (3.26)$$

for the no-slip situation. In the r - z set of coordinates described earlier the free-slip boundary conditions become

Vertical boundaries:

$$u = 0$$

$$\frac{\partial v}{\partial r} = 0$$

$$\frac{\partial p}{\partial r} = \rho g_r \quad (3.27)$$

Horizontal boundaries:

$$\frac{\partial u}{\partial z} = 0$$

$$v = 0$$

$$\frac{\partial p}{\partial z} = \rho g_z \quad (3.28)$$

while the no-slip boundary conditions become

Vertical boundaries:

$$u = 0$$

$$v = 0$$

$$\frac{\partial p}{\partial r} = -\mu \frac{\partial^2 v}{\partial r \partial z} + \rho g_r \quad (3.29)$$

Horizontal boundaries:

$$u = 0$$

$$v = 0$$

$$\frac{\partial p}{\partial z} = -\frac{\mu}{r} \frac{\partial^2 (ru)}{\partial r \partial z} + \rho g_z \quad (3.30)$$

As stated earlier the prescription of boundary conditions at a free surface or interface is by far the most difficult task in a flow simulation of this type. This is partly because the surface does not generally coincide with a coordinate surface, but especially because the reflexive interaction of flow and boundary condition places a heavy responsibility for accuracy and stability on the numerical processes used to implement the boundary condition. This problem is magnified by the presence of surface tension.

Strictly, a free surface refers to an arbitrary surface forming the boundary between a fluid region and a void region. An interface refers to a similar arbitrary surface forming the boundary between two contacting fluid regions. A free surface boundary condition constrains flow variables at the boundary by externally-determined forcing functions (such as atmospheric pressure). Conversely, an interface boundary condition relates flow variables at the boundary in coupled systems of equations. The difference is actually one of application, rather than concept, and the considerations are virtually the same, as far as the boundary condition itself is concerned.

The boundary condition for a free surface is the mathematical equivalent of the statements

1. The fluid pressure at the boundary differs from the external pressure at the boundary by an amount equal to the pressure exerted by the surface tension.
2. The momentum diffusion across the boundary is zero.

Three dependent variables exist in differential form: p , u , and v . Correspondingly, the statements above yield three boundary conditions.

The mathematical equivalent of the first statement is

$$p = p_a + p_s \quad (3.31)$$

where p is the fluid pressure at the boundary, p_a is the external pressure at the boundary (such as atmospheric pressure), and p_s is the so-called surface tension pressure, or force per unit area exerted by surface tension. The problems associated with implementing Equation (3.31) in a finite difference calculation, while not easy, are not insurmountable.

Briefly, the surface tension pressure is computed from Laplace's capillary equation (29),

$$p_s = T_i \kappa \quad (3.32)$$

in which T_i is the surface tension, a property of the fluid, and κ is the curvature of the surface. By definition, the curvature is equal to

$$\kappa = \frac{1}{R_1} + \frac{1}{R_2} \quad (3.33)$$

in which R_1 and R_2 are the radii of curvature of the surface. Much of the discussion in the next chapter is devoted to the accurate computation of κ .

The mathematical equivalent of the second statement was elaborated by Landau and Lifshitz (37) and by Hirt and Shannon (32). The stress, or diffusional momentum flux, at an arbitrary point is given by the pressure tensor,

$$\overline{\overline{P}} = p\overline{\overline{I}} + \overline{\overline{\tau}} \quad (3.34)$$

Each component P_{ij} gives the magnitude of i -coordinate momentum flux diffusing across a plane perpendicular to the j -coordinate axis. If $\overline{n}$ is a unit vector normal to an arbitrary plane then the vector quantity of momentum diffusing across this plane is

$$\overline{\overline{P}} \cdot \overline{n}$$

In two-dimensional Cartesian coordinates the x and y components of this vector are obtained from

$$\begin{aligned}
 \begin{bmatrix} p + \tau_{xx} & \tau_{xy} \\ \tau_{yx} & p + \tau_{yy} \end{bmatrix} \begin{bmatrix} n_x \\ n_y \end{bmatrix} &= \begin{bmatrix} p - 2\mu \frac{\partial u}{\partial x} & -\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\ -\mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & p - 2\mu \frac{\partial v}{\partial y} \end{bmatrix} \begin{bmatrix} n_x \\ n_y \end{bmatrix} \\
 &= \begin{bmatrix} n_x (p - 2\mu \frac{\partial u}{\partial x}) - n_y \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \\ -n_x \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + n_y (p - 2\mu \frac{\partial v}{\partial y}) \end{bmatrix}
 \end{aligned}$$

where n_x and n_y are the components of the unit normal vector. A unit tangent vector is $\bar{t}$ and has components n_y and $-n_x$. The normal and tangential components of the diffusional momentum flux vector are

$$(\bar{P} \cdot \bar{n}) \cdot \bar{n}, \quad (\bar{P} \cdot \bar{n}) \cdot \bar{t}$$

Each must be zero, giving the equations

$$\begin{aligned}
 p - 2\mu \left[n_x^2 \frac{\partial u}{\partial x} + n_x n_y \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + n_y^2 \frac{\partial v}{\partial y} \right] &= 0 \\
 \mu [2n_x n_y - (n_x^2 - n_y^2) \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) - 2n_x n_y \frac{\partial v}{\partial y}] &= 0
 \end{aligned} \tag{3.35}$$

These equations are difficult to implement in a numerical calculation because finite difference approximations of the velocity derivatives require knowledge of undefined velocities at points lying outside the fluid. The original MAC method discarded these equations entirely, instead setting surface pressures to zero and imposing the condition of incompressibility in each surface cell. This is a crude approximation since, strictly speaking, incompressibility should exist only in that portion of a cell actually occupied by fluid. Hirt and Shannon (32) observed that these approximations are adequate except for flows with very low Reynolds numbers. They suggested that if the

surface curvature is small enough to be adequately resolved by the assemblage of surface cells then the approximations

$$\begin{aligned} p - 2\mu \left(\frac{\partial u_n}{\partial n} \right) &= 0 \\ \mu \left(\frac{\partial u_n}{\partial m} + \frac{\partial u_m}{\partial n} \right) &= 0 \end{aligned} \quad (3.36)$$

may be used, where n and m refer to the normal and tangential directions. The derivatives are then approximated with known velocities within the fluid region. This artifice is intended only for simulations of flows without surface tension, and clearly is unsuited to simulations of drops.

In Sandry's (52) MAC simulations of forming and separating drops he used Daly's method (9) to compute the surface tension force and the method of Chan and Street (5) to implement the pressure boundary condition, Equation (3.31). Since these were single-fluid simulations Sandry discarded the normal and tangential stress conditions, Equations (3.35) and forced continuity at the surface, as in the original MAC method. The failure of his program to produce accurate drop profiles near separation attests to the inadequacy of the approximation.

Rather than attempting to devise suitable approximations to the normal and tangential stress conditions because the necessary data are absent, it is better to leave them intact and construct the solution such that the necessary data are routinely computed and made available. This thinking, coupled with the fact that simulations of drops passing through liquid media are likely of greater scientific value than simulations of drops falling in a void, leads one to the conclusion

that the simulation should be constructed as a two-fluid calculation, with both fluid phases incompressible.

In principle any two-fluid problem may be solved using coupled sets of single-fluid calculations, with the coupling being provided by the interfacial boundary condition. The statements for this condition are similar to those of the free-surface condition; they are:

1. The pressure difference between the two fluid regions at the boundary is equal to the interface tension pressure.
2. The velocity and stress at the interface are continuous.

The first condition is essentially the same as the pressure boundary condition described for a free surface and may be written

$$p_1 = p_I + p_2$$

where p_1 and p_2 are the respective fluid pressures at the interface. Since there is no mathematical difference between interfacial tension and surface tension the symbol p_s will be used hereinafter to denote both, and the pressure condition is written

$$p_1 = p_s + p_2 \quad (3.37)$$

The sign convention for p_s is established beforehand, and whichever is used is immaterial, as long as usage is consistent.

The second statement translates to

$$\begin{aligned} \bar{U}_1 &= \bar{U}_2 \\ \bar{P}_1 \cdot \bar{n} &= \bar{P}_2 \cdot \bar{n} \end{aligned} \quad (3.38)$$

Assuming no slip exists at the interface the incompressibility requirement forces continuity of the velocities, and the boundary condition reduces to

$$\bar{p}_1 \cdot \bar{n} = \bar{p}_2 \cdot \bar{n} \quad (3.39)$$

The two-fluid MAC method provides the means of combining computations for both regions with Equation (3.39) in a single calculation, using volume-weighted average properties (ρ and μ) in the vicinity of the interface. The methods of Daly (9) and Chan and Street (5) facilitate implementation of the pressure boundary condition (3.37). The present study provides means of joining the two halves of the problem into a single cohesive, self-consistent algorithm.

That technique makes use of the fact that the momentum equation is linear in pressure. This makes possible the use of the superposition principle in computing the pressure field from a given velocity field at some time. For this purpose it may be reasoned that the velocity and pressure fields satisfy the equations

$$\begin{aligned} \rho_1 \frac{\partial \bar{U}}{\partial t} &= - \rho_1 \bar{\nabla} \cdot (\bar{U}\bar{U}) - \bar{\nabla} p_1 - \mu_1 \bar{\nabla} \times \bar{\nabla} \times \bar{U} + \rho_1 \bar{g} \\ \rho_2 \frac{\partial \bar{U}}{\partial t} &= - \rho_2 \bar{\nabla} \cdot (\bar{U}\bar{U}) - \bar{\nabla} p_2 - \mu_2 \bar{\nabla} \times \bar{\nabla} \times \bar{U} + \rho_2 \bar{g} \end{aligned} \quad (3.40)$$

at respective points in fluid regions 1 and 2, and also satisfy Equations (3.37) and (3.38) at the boundary of the two regions. Equations (3.40) are derived by substituting constant density and viscosity into Equation (3.11). It may now be reasoned that the continuous phase (identified with region 2) actually extends throughout the flow region,

and that the discontinuous phase (identified with region 1) consists of the components

$$\begin{aligned} p_1 &= p_2 + \Delta p \\ \rho_1 &= \rho_2 + \Delta \rho \\ \mu_1 &= \mu_2 + \Delta \mu \end{aligned} \quad (3.41)$$

of pressure, density, and viscosity. Accordingly, we may write

$$\rho_c \frac{\partial \bar{U}}{\partial t} = - \rho_c \bar{\nabla} \cdot (\bar{U}\bar{U}) - \bar{\nabla} p_c - \mu_c \bar{\nabla} \times \bar{\nabla} \times \bar{U} + \rho_c \bar{g} \quad (3.42)$$

for the continuous phase and

$$\begin{aligned} (\rho_c + \Delta \rho) \frac{\partial \bar{U}}{\partial t} &= - (\rho_c + \Delta \rho) \bar{\nabla} \cdot (\bar{U}\bar{U}) - \bar{\nabla} (p_c + \Delta p) - (\mu_c + \Delta \mu) \bar{\nabla} \times \bar{\nabla} \times \bar{U} \\ &\quad + (\rho_c + \Delta \rho) \bar{g} \end{aligned} \quad (3.43)$$

in the discontinuous phase. Subtracting Equation (3.42) from Equation (3.43) gives

$$(\Delta \rho) \frac{\partial \bar{U}}{\partial t} = - (\Delta \rho) \bar{\nabla} \cdot (\bar{U}\bar{U}) - \bar{\nabla} (\Delta p) - (\Delta \mu) \bar{\nabla} \times \bar{\nabla} \times \bar{U} + (\Delta \rho) \bar{g} \quad (3.44)$$

Following the procedure outlined previously, Equations (3.42) and (3.44) may be used to derive two pressure equations:

$$\bar{\nabla} p_c = - \rho_c (Q + \frac{\partial D}{\partial t}) \quad (3.45)$$

$$\bar{\nabla} (\Delta p) = - (\Delta \rho) (Q + \frac{\partial D}{\partial t}) \quad (3.46)$$

To compute the pressure field at time t the unweighted source term $(Q + \partial D / \partial t)$ is computed for the entire region using $\bar{U}(t)$.

Equation (3.45) is solved for the entire region without regard to the phase discontinuity, and the pressure boundary conditions are those in Equations (3.27-3.30) with p_c , ρ_c , and μ_c substituted for p , ρ , and μ . A separate computation produces Δp in the discontinuous phase, using the free surface boundary condition, and using Δp , $\Delta \rho$, and $\Delta \mu$ in the fixed surface boundary conditions. Δp is undefined outside the discontinuous region.

CHAPTER 4. THE FINITE DIFFERENCE

APPROXIMATION AND THE MAC METHOD

The Basic MAC Technique

Before any sort of numerical implementation may be devised the differential equations and boundary conditions must be represented as finite difference equations. The form these take depends on the locations of the velocity and pressure variables. In the MAC method the fluid region is divided into an array or mesh of rectangular cells, each measuring δr by δz . Values of p , Q , and D are located at cell centers, while velocities are located at cell boundaries. This is depicted in Figure 4.1. Although a number of different arrangements are possible, the developers of the MAC method settled on this one after considerable experimentation (62). With velocity mesh points located at cell boundaries, it is a simple matter to compute values of D and p at cell centers using central difference versions of the continuity and pressure equations. Correspondingly, cell-centered values of D and p are easily incorporated into central difference representations of the velocity equations. Also, this placement of velocities is superior to other methods for treatment of boundary information at horizontal and vertical walls and at lines of symmetry.

Superimposed on the cell mesh is the particle grid, a set of movable massless particles whose coordinates change in accordance with local fluid velocity. The purpose of this grid is to permit observation of the motion of the fluid, and to determine the position of the free surface. Early MAC calculations (62) applied no special conditions

Figure 4.1. Locations of field variables in cell ij

at free surfaces, and particles were used primarily for visualization of the fluid. As free surface boundary conditions were added (32), the role of the particle grid gained importance. When surface tension became important it was useful to designate a special sequence of surface or interface particles in order to resolve the position of the free surface accurately and to furnish the curvature of the surface for computing the surface tension pressure (9).

First-order central difference formulas are used to approximate the differential equations and boundary conditions. The velocity divergence 3.16, expanded at cell centers (i, j) , is

$$D_{ij} = \frac{r_{i+\frac{1}{2}} u_{i+\frac{1}{2}j} - r_{i-\frac{1}{2}} u_{i-\frac{1}{2}j}}{r_i \delta r} + \frac{v_{ij+\frac{1}{2}} - v_{ij-\frac{1}{2}}}{\delta z} \quad (4.1)$$

with the requirement

$$D_{ij} = 0$$

for incompressibility in cell (i, j) . The momentum Equations (3.17, 3.18) for constant viscosity are expanded at $(i + \frac{1}{2}, j)$ and $(i, j + \frac{1}{2})$ and at time $n\delta t$ to give

$$\begin{aligned} \frac{1}{\delta t} [(\rho u)_{i+\frac{1}{2}j}^{n+1} - (\rho u)_{i+\frac{1}{2}j}^n] &= \frac{1}{r_{i+\frac{1}{2}} \delta r} [(\rho r u^2)_{ij} - (\rho r u^2)_{i+1j}] \\ &+ \frac{1}{\delta z} [(\rho u v)_{i+\frac{1}{2}j-\frac{1}{2}} - (\rho u v)_{i+\frac{1}{2}j+\frac{1}{2}}] + \frac{1}{\delta r} (p_{ij} - p_{i+1j}) \\ &+ \mu \left[\frac{1}{\delta z^2} (u_{i+\frac{1}{2}j+1} - 2u_{i+\frac{1}{2}j} + u_{i+\frac{1}{2}j}) \right. \\ &\left. - \frac{1}{\delta r \delta z} (v_{i+1j+\frac{1}{2}} + v_{ij-\frac{1}{2}} - v_{i+1j-\frac{1}{2}} - v_{ij+\frac{1}{2}}) + \rho g_r \right] \end{aligned} \quad (4.2)$$

$$\begin{aligned}
\frac{1}{\delta t} [(\rho v)^{n+1}_{ij+\frac{1}{2}} - (\rho v)_{ij+\frac{1}{2}}] &= \frac{1}{r_i \delta r} [(\rho r u v)_{i-\frac{1}{2}j+\frac{1}{2}} - (\rho r u v)_{i+\frac{1}{2}j+\frac{1}{2}}] \\
&+ \frac{1}{\delta z} [(\rho v^2)_{ij} - (\rho v^2)_{ij+\frac{1}{2}}] + \frac{1}{\delta z} (p_{ij} - p_{ij+1}) \\
&+ \frac{\mu}{r_i \delta r} [r_{i-\frac{1}{2}} (\frac{u_{i-\frac{1}{2}j+1} - u_{i-\frac{1}{2}j}}{\delta z} - \frac{v_{ij+\frac{1}{2}} - v_{i-1j+\frac{1}{2}}}{\delta r}) \\
&- r_{i+\frac{1}{2}} (\frac{u_{i+\frac{1}{2}j+1} - u_{i+\frac{1}{2}j}}{\delta z} - \frac{v_{i+1j+\frac{1}{2}} - v_{ij+\frac{1}{2}}}{\delta r})] + \rho g_z \quad (4.3)
\end{aligned}$$

The superscript $n+1$ denotes values at time $(n+1)\delta t$, while the omitted subscript n is understood. Daly (10) gives the more complete approximation of Equations (3.14, 3.15), which allow variable viscosity.

Similarly, the pressure Equation (3.19), expanded at cell centers becomes

$$\begin{aligned}
\frac{1}{r_i \delta r^2} [r_{i+\frac{1}{2}}(p_{i+1j} - p_{ij}) - r_{i-\frac{1}{2}}(p_{ij} - p_{i-1j})] \\
+ \frac{1}{\delta z^2} [p_{ij+1} - 2p_{ij} + p_{ij-1}] = -\rho_\phi (Q_{ij} + \frac{\partial p_{ij}}{\partial t}) \quad (4.4)
\end{aligned}$$

where ρ_ϕ is ρ_c or $\Delta\rho$ depending on whether p is used to denote p_c or Δp and

$$\begin{aligned}
Q_{ij} &= \frac{1}{r_i \delta r^2} [(ru^2)_{i+1j} - 2(ru^2)_{ij} + (ru^2)_{i-1j}] \\
&+ \frac{1}{\delta z^2} [v^2_{ij+1} - 2v^2_{ij} + v^2_{ij-1}] \\
&+ \frac{2}{r_i \delta r \delta z} [(ruv)_{i+\frac{1}{2}j+\frac{1}{2}} + (ruv)_{i-\frac{1}{2}j-\frac{1}{2}} \\
&- (ruv)_{i+\frac{1}{2}j-\frac{1}{2}} - (ruv)_{i-\frac{1}{2}j+\frac{1}{2}}] \quad (4.5)
\end{aligned}$$

It should be noted that whenever any of these formulas requires a variable at a point other than a mesh point a simple average should be

used. For example u_{ij} is replaced by $(u_{i+\frac{1}{2}j} + u_{i-\frac{1}{2}j})/2$.

Before discussing the finite difference forms of the boundary conditions it is necessary to describe the manner in which the MAC method differentiates between various types of interior and boundary cells. Each cell possesses one or more flags or indicators to denote its function and relationship to other cells. The two major divisions are interior cells and boundary cells; a fixed boundary or line of symmetry always passes along the common border of an interior cell and a boundary cell. The major types of flags for interior cells are:

FULL: A cell containing particles and having no adjacent EMP cell neighbors; this flag indicates that the cell lies completely within a fluid region.

EMP: A cell which contains no particles; an EMP cell lies completely outside any fluid region.

SUR: A cell containing particles and has at least one EMP cell neighbor.

In addition to these major flags, interior cells may possess any of the auxiliary flags:

OB: A cell lying adjacent to a boundary cell.

CONT: A FULL or SUR cell lying completely within the continuous phase.

DISC: A FULL or SUR cell lying completely within the discontinuous phase.

INTF: A FULL or SUR cell containing interface particles.

All boundary cells possess the flag BND. In addition they may have any of the following:

FRSLP: A free-slip boundary cell

NOSLP: A no-slip boundary cell

IN: A fluid input cell

OUT: A fluid output cell

EMPBND: An unused boundary cell

FRSLP and NOSLP cells which form the corners of obstacles or walls carry the additional flag COR. IN and OUT cells allow the definition of passages for fluid to be added or removed from the system. Figure 4.2 shows an arbitrary fluid region, demonstrating the types and purposes of the various cells. It should be noted that the flags CONT, DISC, and INTF, represent extensions to the original MAC method (62); the reasons for these will become apparent in the next section when the modifications to the original two-fluid MAC method, necessary for this work, are disclosed.

The finite difference boundary conditions are written such that field variables or their derivatives are located at the common boundary of a BND cell and an interior cell. This is illustrated in Figure 4.3. The free-slip and no-slip conditions are, for vertical boundaries,

Free slip:

$$\frac{(p_c)_{i+1j} - (p_c)_{ij}}{\delta r} = \rho_c g_r$$

$$\frac{(\Delta p)_{i+1j} - (\Delta p)_{ij}}{\delta r} = \Delta \rho g_r \quad (4.6)$$

$$u_{i+\frac{1}{2}j} = 0$$

$$v_{ij+\frac{1}{2}} = v_{i+1j+\frac{1}{2}}$$

Figure 4.2. Arbitrary fluid region, showing various types of cells

Figure 4.3. Cells at horizontal and vertical walls

$$v_{ij-\frac{1}{2}} = v_{i+1j-\frac{1}{2}}$$

No-slip:

$$\begin{aligned} \frac{(p_c)_{i+1j} - (p_c)_{ij}}{\delta r} &= \frac{2\mu}{\delta r \delta z} (v_{ij+\frac{1}{2}} - v_{ij-\frac{1}{2}}) + \rho_c g_r \\ \frac{(\Delta p)_{i+1j} - (\Delta p)_{ij}}{\delta r} &= \Delta \rho g_r \end{aligned} \quad (4.7)$$

$$u_{i+\frac{1}{2}j} = 0$$

$$v_{ij+\frac{1}{2}} = -v_{i+1j+\frac{1}{2}}$$

$$v_{ij-\frac{1}{2}} = -v_{i+1j-\frac{1}{2}}$$

and for horizontal boundaries,

Free-slip:

$$\begin{aligned} \frac{(p_c)_{ij+1} - (p_c)_{ij}}{\delta z} &= \rho_c g_z \\ \frac{(\Delta p)_{ij+1} - (\Delta p)_{ij}}{\delta z} &= \Delta \rho g_z \end{aligned} \quad (4.8)$$

$$u_{i-\frac{1}{2}j} = u_{i-\frac{1}{2}j+1}$$

$$u_{i+\frac{1}{2}j} = u_{i+\frac{1}{2}j+1}$$

$$v_{ij+\frac{1}{2}} = 0$$

No-slip:

$$\begin{aligned} \frac{(p_c)_{ij+1} - (p_c)_{ij}}{\delta z} &= \frac{\partial \mu}{\partial r \partial z} [(ru)_{i+\frac{1}{2}j} - (ru)_{i-\frac{1}{2}j}] + \rho_c g_z \\ \frac{(\Delta p)_{ij+1} - (\Delta p)_{ij}}{\delta z} &= \Delta \rho g_z \end{aligned} \quad (4.9)$$

$$u_{i-\frac{1}{2}j} = -u_{i-\frac{1}{2}j+1}$$

$$u_{i+\frac{1}{2}j} = -u_{i+\frac{1}{2}j+1}$$

$$v_{ij+\frac{1}{2}} = 0$$

Boundary conditions for IN and OUT cells require special tailoring to fit the type of flow they are used to induce. In the original MAC method these were derived such that velocity through a port would be a free parameter, with boundary pressure varying to satisfy the momentum equations. In this work it is more natural to let pressure be the flow-inducing parameter, with velocity being forced to satisfy continuity. For both IN and OUT cells the boundary cell pressure is set to

$$p = p_{\text{ext}} \quad (4.10)$$

where p_{ext} is some externally controllable pressure. For horizontal boundaries the conditions for the two types of cell are

$$\begin{aligned} \text{IN: } u &= 0, \quad u_{i+\frac{1}{2}j} = -u_{i+\frac{1}{2}j+1} \\ \frac{\partial v}{\partial z} &= 0, \quad v_{ij+\frac{1}{2}} = v_{ij-\frac{1}{2}} \end{aligned} \quad (4.11)$$

$$\begin{aligned} \text{OUT: } \frac{\partial u}{\partial z} &= 0, \quad u_{i+\frac{1}{2}j} = u_{i+\frac{1}{2}j+1} \\ \frac{\partial v}{\partial z} &= -\frac{1}{r} \frac{\partial(ru)}{\partial r}, \quad \frac{v_{ij+1} - v_{ij-\frac{1}{2}}}{\delta z} = -\frac{(ru)_{i+\frac{1}{2}j} - (ru)_{i-\frac{1}{2}j}}{r_i \delta r} \end{aligned} \quad (4.12)$$

The conditions for vertical boundaries are completely analogous.

With the necessary mathematical groundwork laid, the general strategy used by the MAC method for simultaneously solving the continuity and momentum equations may be stated. The specific modifications of

the technique necessary for this study primarily concern the interface boundary condition; discussion of these is reserved for the next section.

Motion of the fluid in a MAC calculation is made apparent by the changes in positions of particles from time to time. It is natural to make these changes at discrete points along the time axis; therefore the simulation, beginning at $t = 0$, proceeds in a sequential motion-picture-frame fashion. Changes in the velocity field are governed by the finite difference forms of the momentum Equations (4.2, 4.3). As a consequence of the continuity requirement, with each successive velocity field is associated a unique pressure field which must satisfy the pressure Equation (4.4). The particular way in which the continuity equation is combined with the pressure equations constitutes an essential part of the MAC method. Considering that the computed velocity field at time $n\delta t$ is the result of numerical processes which occurred at $(n-1)\delta t$, it is certain that the velocities do not satisfy continuity perfectly, i.e., the actual divergence, D , may differ from zero. The solution process applies a correction by computing D at $n\delta t$ and using it in the calculation of the velocities at $(n+1)\delta t$ such that the condition $D = 0$ at $(n+1)\delta t$ is sought. To accomplish this the time derivative of D in the pressure equation is expanded so that

$$\nabla^2 p = -\rho_\phi \left(Q + \frac{D_{n+1} - D_n}{\delta t} \right)$$

where D_n and D_{n+1} are divergences at $n\delta t$ and $(n+1)\delta t$. The continuity equation is used to set $D_{n+1} = 0$ giving

$$\nabla^2 p = -\rho_\phi (Q - D/\delta t) \quad (4.13)$$

in which the subscript n is dropped. This process is simply the application of negative feedback to eliminate drift caused by accumulated numerical errors, and gives the MAC method its characteristic ability to maintain long-term stability.

Equation (4.13) is solved at $n\delta t$ by the relaxation method which proceeds by repeatedly scanning the pressure field, each time replacing the pressure at each point by an average of the pressures at its four neighbors and a source function of position. The two pressure equations may be written in the form

$$\nabla^2 p_c = (S_c)_{ij} \quad (4.14)$$

$$\nabla^2 (\Delta p) = (S_\Delta)_{ij} \quad (4.15)$$

or, generally,

$$\nabla^2 p = S_{ij}$$

where S_{ij} is the appropriate source function.

Expanding in finite difference form,

$$\begin{aligned} \frac{1}{r_i \delta r^2} [r_{i+\frac{1}{2}}(p_{i+1j} - p_{ij}) - r_{i-\frac{1}{2}}(p_{ij} - p_{i-1j})] \\ + \frac{1}{\delta z^2} [p_{ij+1} - 2p_{ij} + p_{ij-1}] = S_{ij} \end{aligned}$$

Letting $\delta r = \delta z = \delta x$ and solving for p_{ij} ,

$$p_{ij} = \frac{1}{4} \left[\left(\frac{r_{i+\frac{1}{2}}}{r_i} \right) p_1 + \left(\frac{r_{i-\frac{1}{2}}}{r_i} \right) p_3 + p_2 + p_4 - S_{ij} \delta x^2 \right] \quad (4.16)$$

where

$$p_1 = p_{i+1j}$$

$$p_2 = p_{ij+1}$$

$$p_3 = p_{i-1j}$$

$$p_4 = p_{ij-1}$$

Equation (4.16), along with the appropriate finite difference boundary conditions, is used to determine the relaxed pressure field. At the beginning of each pass through the field the boundary conditions are used to estimate pressures at the centers of the boundary cells from the current pressures in adjacent interior cells, or from external pressures. Then, each internal cell pressure is replaced with one computed from Equation (4.16). A new pass is begun by reestimating the boundary cell pressures, and so on until the pressure corrections from one iteration to the next are less than some prescribed tolerance.

Some authors suggest attempting to increase the speed of convergence by using a so-called overrelaxation parameter α (38, p. 149) such that the iteration formula is in the form

$$p_{ij} = p_{ij} + \alpha \left[\left(\frac{r_{i+\frac{1}{2}}}{r_i} \right) p_1 + \left(\frac{r_{i-\frac{1}{2}}}{r_i} \right) p_3 + p_2 + p_4 - 4p_{ij} - S_{ij} \delta x^2 \right] \quad (4.17)$$

where α varies from 0.25 to 0.50. Note that Equation (4.17) reduces to Equation (4.16) when $\alpha = 0.25$. For any coordinate system other than Cartesian the optimum value of α must be determined by experiment; no such attempt has been made in this study, but the value 0.33 for α appears to shorten convergence time considerably over the value 0.25.

The relaxed pressure field is used to supply the pressure gradients in the momentum equations. Other accelerations stem from body force,

which is applied directly, and from viscous and convective effects, which are computed from velocity and then applied. Note that, when two fluids are present, allowance must be made in Equations (4.2, 4.3) for varying cell densities in the time derivatives and convective terms. The density of any cell which straddles the phase boundary must be computed as a volume-weighted average of the individual fluid densities. In the original two-fluid MAC method, this is done by employing two types of particles, one to mark each fluid region. Cell densities are computed by tallying the numbers of each type of particle lying within the cells. This method requires the use of a great many particles in order to achieve reasonable resolution, and was scrapped in this study in favor of one which computes densities directly from the shape of the interface. This technique results in considerable savings of memory and is described in the next section.

It should be noted that cell density information is needed not only at $n\delta t$ but at $(n+1)\delta t$ as well. Since this "advanced time" information is not known at the "present time," it must be determined by iteration. The present densities are used as estimates for the advanced densities, and the advanced velocities are computed. The advanced particle positions are then determined and used to compute revised estimates of advanced density, and the process continues until convergence. In the original two-fluid MAC method one full pressure calculation is required for every density iteration. However, in the modification used for this study computation of neither p_c nor Δp requires any average cell density information. Consequently, both

pressure calculations may be completed before the start of the density iteration, thereby saving considerable computing time.

When the density iteration is complete both advanced densities and advanced velocities are known. The time step is completed by advancing time by δt and moving the particles to new positions with the advanced velocities. At this point, plots may be made, results printed, and any other mechanical function performed.

At the completion of the time step the cellular divergences, D_{ij} , may be calculated from the latest velocity information. This array is a reliable barometer of the performance of a fluid flow simulation since it is easily monitored and is supposed to tend to zero.

Specific Modifications for This Study

The key modifications necessary for this work concern the most elusive numerical problem: The free surface boundary condition. As discussed in the last chapter, the MAC method's greatest claim to success is, ironically, also its greatest weakness: The poorest approximations are made at the free surface. By dint of the arguments made earlier it is possible in a two-fluid calculation to sidestep the viscous stress boundary conditions entirely and concentrate on the pressure boundary condition.

Fortunately, this problem is tractable, as evidenced by the successful previous applications of the MAC method to problems characterized by the presence of surface tension or interfacial tension (10, 52). The problem consists of three parts:

1. A suitable representation of the surface or interface must be devised.
2. Means must be established for computing the surface tension pressure, or pressure difference across the phase boundary due to surface or interfacial tension.
3. The surface tension pressure must be applied to the calculation of pressures or velocity changes.

Daly (9) has proposed that an independent sequence of particles be used to represent the interface curve. Since this curve is not generally monotonic it is to be subdivided into a set of monotonic subsequences. To each subsequence is fitted a set of cubic splines whose first and second derivatives are used to compute the surface tension pressure. This is converted into a set of accelerations and added to the momentum equations at the velocity points nearest the interface.

The method of Chan and Street (5) incorporates a somewhat different approach for single-fluid calculations. Recognizing that it is improper to apply a surface pressure at a cell center any distance from the surface, they have modified the relaxation formula to allow irregularly spaced data to be used at so-called "irregular stars." Referring to Figure 4.4, their relaxation formula computes the center pressure p_0 based on pressures $p_1 - p_4$ and arms $\alpha_1 - \alpha_4$. In this approach, if surface tension is applied at the pressure points on the surface it is felt throughout the pressure field, and is thereby reflected in the velocity changes.

Figure 4.4. Irregular star

This method is somewhat awkward to apply directly to a two-fluid problem because the pressures at cell centers across the phase boundary (p'_2 and p'_3 in Figure 4.4) must be used in addition to surface tension pressures p_2 and p_3 in the determination of p_0 . The derivation of the relaxation formula inevitably requires knowledge of two components of p_0 : one due to unperturbed pressures existing throughout the fluid region, and the other due to the surface tension discontinuity. This fact alone mandates the use of the two pressure fields p_c and Δp , described previously.

In his single-fluid studies of drops Sandry (52) combined these two techniques, adding some modifications of his own. Particularly, he found it more convenient to express interface points (r, z) as functions of a parameter x , than to break the interface curve into monotonic subsequences. All fitting and smoothing operations were then performed individually on the functions $r(x)$ and $z(x)$. Since arc length along a curve from some starting point is mathematically a suitable parameter for a curve, he chose to use its numerical approximation, cumulative chord length from particle to particle.

The procedure is illustrated with the fit of $r(x)$; the process is mutatis mutandis the same for $z(x)$. The cubic spline fit is based on the linear definition for interpolated values of the second derivative

$$r''(x) = M_{k-1} \frac{x_k - x}{l_k} + M_k \frac{x - x_{k-1}}{l_k} \quad (4.18)$$

where M_{k-1} , M_k are the second derivatives of $r(x)$ at the particle positions for x_{k-1} , x_k , and l_k is the chord length $x_k - x_{k-1}$. Note that

$$l_k = [(r_k - r_{k-1})^2 + (z_k - z_{k-1})^2]^{1/2} \quad (4.19)$$

Equation (4.18) is integrated twice with the conditions $r(x_{k-1}) = r_{k-1}$ and $r(x_k) = r_k$ to obtain

$$\begin{aligned} r'(x) = & -M_{k-1} \frac{(x_k - x)^2}{2l_k} + M_k \frac{(x - x_{k-1})^2}{2l_k} \\ & + \frac{r_k - r_{k-1}}{l_k} - \frac{(M_k - M_{k-1})l_k}{6} \end{aligned} \quad (4.20)$$

$$\begin{aligned} r(x) = & M_{k-1} \frac{(x_k - x)^3}{6l_k} + M_k \frac{(x - x_{k-1})^3}{6l_k} \\ & + \left(\frac{r_k}{l_k} - \frac{M_k l_k}{6}\right)(x - x_{k-1}) + \left(\frac{r_{k-1}}{l_k} - \frac{M_{k-1} l_k}{6}\right)(x_k - x) \end{aligned} \quad (4.21)$$

The constants M_k are determined by specifying that $r'(x_{k-1}^-) = (x_{k-1}^+)$, i.e., that the first derivatives of the constructed curve be continuous at the knots. This yields the recursive equation

$$\frac{l_k}{6} M_{k-1} + \frac{l_k + l_{k+1}}{3} M_k + \frac{l_{k+1}}{6} M_{k+1} = \frac{r_{k+1} - r_k}{l_k} - \frac{r_k - r_{k-1}}{l_k} \quad (4.22)$$

The complete set of simultaneous equations may be placed in the matrix

$$\begin{bmatrix} (l_1 + l_2)/3 & l_2/6 & 0 & \cdots & 0 \\ l_2/6 & (l_2 + l_3)/3 & l_3/6 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & l_{k^*}/6 & (l_{k^*} + l_{k^*+1})/3 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ \vdots \\ M_{k^*} \end{bmatrix}$$

$$= \begin{bmatrix} (r_2 - r_1)/\ell_2 - (r_1 - r_0)/\ell_1 - \ell_1 M_0/6 \\ (r_3 - r_2)/\ell_3 - (r_2 - r_1)/\ell_2 \\ \vdots \\ (r_{k^*+1} - r_{k^*})/\ell_{k^*+1} - (r_{k^*} - r_{k^*-1})/\ell_{k^*} - \ell_{k^*+1} M_{k^*+1}/6 \end{bmatrix} \quad (4.23)$$

in which the interface particles are numbered from 1 near the apex of the drop to k^* near the base. To assist with the construction, there is a fictitious particle k_0 which is the reflection of k_1 through the central axis. Also there is particle k^*+1 to denote the base of the drop; its position never changes during the simulation. Before 4.23 can be solved for $M_1, \dots, M_{k^*}$ the end point constants M_0 and M_{k^*+1} must be stated. This requires some caution because errors in these constants produce ripples in $r'(x)$ near the ends of the sequence. M_0 may be eliminated from 4.23 by the relation $r(x_0) = -r(x_1)$, and in the z -fit by the relation $z(x_0) = z(x_1)$. M_{k^*+1} is most easily demonstrated by fitting a cubic to the points (x_k, r_k) or (x_k, z_k) for $k = k^* - 2, \dots, k^* + 1$ and evaluating the second derivative of the cubic at x_{k^*+1} .

Daly solves the matrix Equation (4.23) for $M_1, \dots, M_{k^*}$ using the Thomas algorithm for tridiagonal matrices. This has been found to be too unreliable in this work since, under conditions of close or irregular particle spacing, the second derivatives can fluctuate wildly from knot to knot. This is true even after following his dictum of smoothing each particle found in violation of a "smoothness criterion."

A completely reliable fitting procedure for this study has been the following:

1. Redistribute the particles to a spacing of about one half cell width.
2. Smooth each particle position using a least-squares cubic fit to its ten nearest neighbors. The Forsythe method for fitting polynomials is simple, reliable, and sufficiently economical for this task (38, p. 335).
3. Compute M_k at each point by evaluating the second derivative of the least squares cubic centered at that point.
4. Smooth the sequence $M_1, \dots, M_k$ using least-squares cubics.

With the interface curve fitted by this procedure the surface tension pressure may be computed and applied to the pressure calculation. To do this each cell is checked for its proximity to the interface. Cells whose centers lie within one cell width of the interface are irregular stars, and those whose centers lie within the discontinuous phase are used in applying the surface tension pressure boundary condition. At the end of each short arm the surface tension pressure (p_2 and p_3 in Figure 4.4) is computed using

$$p_s = T_i \left(\frac{r'z'' - z'r''}{[(r')^2 + (z')^2]^{3/2}} + \frac{z'}{r[(r')^2 + (z')^2]^{1/2}} \right) \quad (4.24)$$

This is just Laplace's pressure balance with the curvatures defined in terms of the parametric functions; it is presented by Daly (9) and adapted to cylindrical coordinates by Sandry (52). The derivatives are evaluated using Equations (4.18) and (4.20).

In order to incorporate the values of p_s in computation of Δp the Poisson equation is expanded for unequal arms to give

$$\begin{aligned} \nabla^2 (\Delta p) = & \frac{1}{r_i \delta r} \left[r_{i+\frac{1}{2}} \left(\frac{p_1 - p_o}{\alpha_1} \right) - r_{i-\frac{1}{2}} \left(\frac{p_3 - p_o}{\alpha_3} \right) \right] \\ & + \frac{1}{\delta z} \left[\frac{p_2 - p_o}{\alpha_2} - \frac{p_o - p_4}{\alpha_4} \right] = S_{ij} \end{aligned} \quad (4.25)$$

where

$$\begin{aligned} p_o &= \Delta p_{ij} & p_3 &= \Delta p_{i-1j} \\ p_1 &= \Delta p_{i+1j} & p_4 &= \Delta p_{ij-1} \\ p_2 &= \Delta p_{ij+1} \end{aligned}$$

This formula is based on the notion that equally-spaced data could give rise to the same first derivatives as unequally-spaced data.

Solving for p_o with $\delta r = \delta z = \delta x$,

$$p_o = \left(\sum_{m=1}^4 c_m \right)^{-1} \left(\sum_{m=1}^4 c_m p_m - S_{ij} \delta x \right) \quad (4.26)$$

where

$$\begin{aligned} c_1 &= \frac{r_{i+\frac{1}{2}}}{r_i \alpha_1} & c_2 &= \frac{1}{\alpha_2} \\ c_3 &= \frac{r_{i-\frac{1}{2}}}{r_i \alpha_3} & c_4 &= \frac{1}{\alpha_4} \end{aligned}$$

To use Equation (4.26) mesh point pressures are substituted for p_m when $\alpha_m = \delta x$, and the computed values of p_s are substituted for p_m at the short arms. To guard against the possibility of overflow while computing α_m^{-1} , p_o is simply replaced by p_s on the short arm whenever the interface passes very close (such as within $10^{-3} \delta x$) to the cell center.

Using this method accelerations imparted by the surface tension pressure are distributed throughout the discontinuous phase. One might

well ask how can fluid on only one side of the interface experience an acceleration? Or what is the difference between adding a surface tension acceleration to the fluid on one side of the phase boundary and subtracting (algebraically) it from the fluid on the other side? The answer seems to be that, in the long run, it makes little or no difference. This thinking follows from the incompressible nature of the flow: any acceleration appearing on one side of a cell split by the interface will be transmitted, more or less, to the other side, and then to the rest of the fluid region. Any unbalanced acceleration on one boundary of an interface cell causing a compression or rarefaction during a time step will cause the continuous pressure field, p_c , to react in subsequent time steps to distribute the acceleration on the opposite side of the interface. For adequately short time steps this reaction is fast enough that errors produced by the delay are minor.

It was noted earlier that the high-resolution interface used in this work makes it possible to compute interface cell densities directly from geometrical considerations, rather than having to keep a large inventory of particles just for this purpose. The scheme is based on the assumption that the slope of the interface curve changes only minutely across the span of the cell. Figure 4.5 illustrates the two possible situations: a steep curve and a gently sloping curve passing through an interface cell. In the density averaging process the cell is filled with a rectangular array of fictitious particles. In order to do this, a polynomial is fitted to either $r = r(z)$ or $z = z(r)$, depending on whether the curve is steep or gradual. The numbers of

Figure 4.5. Steep and gradual interface curves through an interface cell

fictitious particles on each side of the curve are tallied and used to compute a volume-weighted average density for the cell.

Illustrating with the second case, in which the curve is represented by $z = p(r)$, the ordinate of each fictitious particle is tested against the computed value of $p(r_0)$, where r_0 is its abscissa. The tallying process is simply a numerical integration. For a cell measuring δr by δz , an element of area is

$$dA = dr dz$$

an element of volume is

$$dV = 2\pi r dA$$

and an element of mass is

$$\begin{aligned} dm &= \rho dV \\ &= 2\pi r \rho dA \end{aligned}$$

where ρ is the local fluid density. The total mass and total volume of the cell are

$$m = \int_C 2\pi r \rho dA$$

$$V = \int_C 2\pi r dA$$

where C denotes the region occupied by the cell, and the average density is

$$\rho_{\text{avg}} = \frac{m}{V} = \frac{(\int_C \rho r dA)}{(\int_C r dA)} \quad (4.27)$$

The denominator in this expression is

$$\int_C r dA = r_m \delta A$$

where r_m is the radius of the cell center and δA is the area of the cell. Also the integral in the numerator may be split into integrals over the subregions C_1 and C_2 separated by the interface curve to give

$$\begin{aligned} \int_C \rho r dA &= \int_{C_1} \rho_1 r dA + \int_{C_2} \rho_2 r dA \\ &= \rho_1 \int_{C_1} r dA + \rho_2 \int_{C_2} r dA \end{aligned}$$

The numerical approximation is made by stating that each element of area is represented by a particle located at its center. If the particle is in C_1 then the entire element dA is in C_1 , and conversely for C_2 . Consequently the integral may be replaced by the approximation

$$\rho_1 \sum_{i=1}^{N_1} (r dA)_i + \rho_2 \sum_{j=1}^{N_2} (r dA)_j$$

where i denotes particles in C_1 , j denotes particles in C_2 , and N_1 , N_2 are the numbers of particles in the two subsets. Recombining numerator and denominator in 4.27 gives

$$\rho_1 \frac{1}{r_m \delta A} \sum_{i=1}^{N_1} (r dA)_i + \rho_2 \frac{1}{r_m \delta A} \sum_{j=1}^{N_2} (r dA)_j$$

which is

$$\rho_1 \left(\frac{dA}{\delta A} \right) \sum_{i=1}^{N_1} \left(\frac{r}{r_m} \right)_i + \rho_2 \left(\frac{dA}{\delta A} \right) \sum_{j=1}^{N_2} \left(\frac{r}{r_m} \right)_j$$

Replacing $(dA/\delta A)$ by its equivalent, $1/N$ where N is the total number of fictitious particles in the cell ($N = N_1 + N_2$), the average cell

density may be written in the form of the weighted average

$$\rho_{\text{avg}} = \left[\frac{1}{N} \sum_{i=1}^{N_1} \left(\frac{r}{r_m} \right)_i \right] \rho_1 + \left[\frac{1}{N} \sum_{j=1}^{N_2} \left(\frac{r}{r_m} \right)_j \right] \rho_2 \quad (4.28)$$

The task of determining whether ρ_1 should be ρ_d or ρ_c (and conversely for ρ_2) is purely a mechanical one, based on the design of the program, and is irrelevant to the discussion.

In a similar vein, the manner of determining the densities of non-interface interior cells requires careful consideration, but is also purely a mechanical problem. As with the original two-fluid MAC method this may be done by tallying large numbers of particles, but that can be avoided, as with the interface cells, by using the interface itself. The problem is basically one of determining which of two regions contains the center of a cell. If a cell center lies within the discontinuous fluid region it is assigned the density ρ_d , otherwise ρ_c .

By its nature the discontinuous fluid region is bounded by a closed contour which, for the drop in Figure 4.6, consists of the interface curve, the base of the drop, and the z-axis. Cells whose centers lie at least one cell width away from all interface cells may be resolved simply by interrogating the cell's current flag, since the interface cannot cross into that cell in any one time step. The cell density is determined to be that for the fluid which completely fills the cell.

The only other cells are those which are proximate to the interface, but through which the interface does not pass. Means for resolving these cells may be established by considering the construction

Figure 4.6. Construction for resolving cell centers lying near the interface. Inset: clockwise shift from P_1 to P_2 around q

shown in Figure 4.6. Interface particles are numbered consecutively starting at the interface. Consequently, motion along the interface from the apex toward the base will subtend clockwise rotation at a point lying near the interface and inside the discontinuous region, and will subtend counterclockwise rotation at a point lying inside the continuous region. Accordingly, for each cell center to be tested (point q in the inset) the two nearest interface particles are examined to determine whether a shift from P_1 to P_2 produces clockwise or counterclockwise motion with respect to q . The details are based on simple trigonometry, and will not be elaborated.

The ultimate purpose of these pressure and density manipulations is the production of local fluid accelerations according to the momentum equation. Accordingly, these data must be applied to the finite difference form of the momentum equation to compute the accelerations. Recalling Equations (4.2, 4.3), there are four types of terms to consider: convective, pressure, viscous, and gravitational. Density appears in the convective and gravitational accelerations and in the time derivatives. One of the special modifications for this study pertains to the way density is handled in the momentum equations.

In the original two-fluid MAC method the local fluid density evaluated at a cell center is always the computed average density of the cell, while the density evaluated at a velocity point is always the average of the two adjacent cell densities. Experience with the sharp phase boundary used in this study has shown that average densities should be applied only to the time derivatives and the convective terms.

The pressure and gravitational terms have a special relationship to each other: they must partially balance each other at every point. In the hydrostatic situation they must exactly balance each other. This may be seen by writing the momentum Equation (3.11) with no fluid motion,

$$\frac{\partial(\rho \bar{U})}{\partial t} = -\bar{\nabla} p + \rho \bar{g} = 0 \quad (4.29)$$

in which convective and viscous terms vanish. In preliminary simulations of stable drops this equation failed to hold in the interface cells. This was attributed to the fact that the pressure was defined such that it possess a sharp discontinuity with gently varying derivatives, while the average local density would be continuous with rapidly varying derivatives. This incompatibility produced artificial accelerations which could not be controlled.

The solution was to incorporate both the pressure and density discontinuities into the calculation. At every velocity point lying within the discontinuous fluid the pressure derivative is

$$\frac{\partial(p + \Delta p)}{\partial r} \text{ or } \frac{\partial(p + \Delta p)}{\partial z}$$

and density ρ_d should be used in place of the computed average density. At points outside this region

$$\frac{\partial p_c}{\partial r} \text{ or } \frac{\partial p_c}{\partial z}$$

and ρ_c should be used. This interpretation is closer to physical reality and produces small errors due only to the finite word size of the machine.

One special precaution must be taken when computing accelerations from the pressure field inside the discontinuous region near the interface. Referring to Figure 4.7, one may compute the derivative using the approximation

$$\frac{\partial(\Delta p)}{\partial r} \approx \frac{p_s - \Delta p_{ij}}{\alpha_1}$$

but when α_1 is small errors left in the values of Δp_{ij} may be greatly magnified. It has been found much safer to use the approximation

$$\frac{\partial(\Delta p)}{\partial r} \approx \frac{p_s - \Delta p_{i-1j}}{\delta r + \alpha_1}$$

which includes an adjacent cell pressure (Δp_{i-1j}) to increase stability.

With these revisions having been considered it is now possible to state the algorithm used to advance from one time frame to the next in the modified MAC method used in this work:

1. Respace and smooth the interface particles, then compute and smooth M_k for $r(x)$ and $z(x)$.
2. Compute surface tension pressure at grid crossings on the interface using the fitted $r(x)$ and $z(x)$.
3. Compute Q and D for each interior cell.
4. Relax p_c and Δp fields.
5. Approximate ρ_{n+1} with ρ_n .
6. Compute u_{n+1} , v_{n+1} .
7. Compute new interface particle positions.
8. Compute updated ρ_{n+1} from the new interface. Compare to old ρ_{n+1} and go to 6 if not converged.

Figure 4.7. Computing pressure accelerations near the interface

9. Move particles to updated positions using u_{n+1} , v_{n+1} . Advance time by δt .
10. Reflag cells to reflect updated particle positions.
11. Create/destroy particles moving into/out of the fluid region.
12. Print results, draw plots.
13. Go to 1 for next time step.

It should be noted that both pressure fields are known before the density loop (steps 6, 7, and 8) is entered. The original two-fluid MAC algorithm required a pressure relaxation within the density loop, thereby requiring more time for convergence.

Initial Conditions

In this study simulations always begin with stable drops, i.e. drops at rest and in mechanical equilibrium. The drops are somehow perturbed early in the simulation, causing them to become unstable. The theory of equilibrium drop profiles has been covered in detail by several authors cited in Chapter 2. It is worthwhile to present a summary here.

A stable pendant drop consists of a discontinuous phase hanging within a continuous phase. The characteristic profile stems from the requirement that the pressures inside and outside the drop be hydrostatic, i.e. vary linearly with depth. Figure 4.8 shows a typical profile and depicts the coordinate systems used. It is convenient to develop the profile using the r - y system and then transform to the r - z system. In the convention for body forces used here gravity acts

Figure 4.8. Variables and coordinate systems used to generate the initial profile

downward, while the discontinuous phase is buoyed upward by the denser continuous phase.

Recalling from Chapter 3 the requirement for a hydrostatic pressure field is

$$\bar{\nabla} p = \bar{\rho} \bar{g} \quad (4.30)$$

Writing this for each homogeneous region,

$$\bar{\nabla} p_c = \rho_c \bar{g}$$

$$\bar{\nabla} p_d = \rho_d \bar{g}$$

With no radial component of pressure gradient or gravity this becomes

$$\frac{dp_c}{dz} = \rho_c g$$

$$\frac{dp_d}{dz} = \rho_d g$$

Integrating from the arbitrary reference plane $z = z_o$ at which $p_c = p_{co}$ and $p_d = p_{do}$,

$$p_c - p_{co} = \rho_c g(z - z_o)$$

$$p_d - p_{do} = \rho_d g(z - z_o) \quad (4.31)$$

In Figure 4.8 the reference plane is the apex so that $z - z_o = y$. Thus

$$p_c = p_{co} + \rho_c g y$$

$$p_d = p_{do} + \rho_d g y \quad (4.32)$$

Subtracting these equations,

$$(p_d - p_c) = (p_{do} - p_{co}) + (\rho_d - \rho_c)gy$$

But $p_d - p_c$ is the pressure difference p_s at the interface and $\rho_d - \rho_c$ is the density difference $\Delta\rho$. Thus

$$p_s = p_{so} + \Delta\rho gy \quad (4.33)$$

where p_{so} is the pressure difference at the interface. Laplace's pressure balance is

$$p_s = T_i \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

which, at the apex, becomes

$$p_{so} = \frac{2T_i}{R_o} \quad (4.34)$$

where R_o is the radius of curvature at the apex. Eliminating p_s and p_{so} in Equation (4.33) produces

$$T_i \left(\frac{1}{R_1} + \frac{1}{R_2} \right) = \frac{2T_i}{R_o} + \Delta\rho gy \quad (4.35)$$

Using arc length along the interface curve from the apex as a parameter we may define the angle ϕ such that

$$\frac{dy}{ds} = \sin \phi$$

$$\frac{dx}{ds} = \cos \phi \quad (4.36)$$

where

$$ds^2 = dx^2 + dy^2$$

It is easily shown (18, p. 57) that the radii of curvature are

$$R_1 = \frac{ds}{d\phi}$$

$$R_2 = \frac{x}{\sin \phi}$$

Substituting these into the pressure balance,

$$T_i \left(\frac{d\phi}{ds} + \frac{\sin \phi}{x} \right) = \frac{2T_i}{R_o} + \Delta \rho g y$$

which may be placed in the form

$$\frac{d\phi}{ds} = \frac{\Delta \rho g}{T_i} y - \frac{\sin \phi}{x} + \frac{2}{R_o} \quad (4.37)$$

This equation may be normalized by placing in the form

$$\frac{d\phi}{ds_n} = \frac{\Delta \rho g R_o^2}{T_i} y_n - \frac{\sin \phi}{x_n} + 2 \quad (4.38)$$

where

$$s_n = \frac{s}{R_o}$$

$$x_n = \frac{x}{R_o}$$

$$y_n = \frac{y}{R_o}$$

The quantity $\Delta \rho g R_o^2 / T_i$ is a dimensionless group called the Bond number Bo , used in studies of interfacial phenomena. Inspection of Equation (4.38) shows that the shape of the drop is governed entirely by Bo , while its size is controlled exclusively by R_o .

To use Equation (4.38) to generate drop profiles one begins by initializing

$$\phi = 0$$

$$x_n = y_n = s_n = 0$$

at the apex. Equations (4.36) and (4.38) are numerically integrated in simultaneous fashion until the desired base radius or contact angle is attained. The Runge-Kutta method is ideal for this task. One pitfall is that $\sin \phi / x_n$ has the limiting form $0/0$ at the apex. However, application of de L'Hospital's rule shows that

$$\lim_{s_n \rightarrow 0} \frac{\sin \phi}{x_n} = 1$$

and this is the value used to begin the integration.

The formulation of the initial conditions is made complete by specifying the initial pressures and velocities. The pressures are computed using Equations (4.31), and the velocities are all set to zero.

Stability and Accuracy

In their original disclosure (62) the developers of the MAC method suggested two limitations on the size of the time step. One is analogous to the Courant condition for compressible flow calculations and is based on the speed of waves in a tank. This is

$$c \delta t < \frac{2 \delta r \delta z}{\delta r + \delta z} \quad (4.39)$$

where

$$c = \left[\frac{g}{k} \tanh(kh) \right]^{1/2}$$

and c is the wave speed, k is the wave number, and h is the height of fluid in the tank. For square cells this requirement specifies that

the wave move by not more than one cell width in a time step. The other condition is

$$2\nu\delta t < \frac{\delta x^2 \delta z^2}{\delta x^2 + \delta z^2} \quad (4.40)$$

where $\nu = \mu/\rho$ is the kinematic viscosity. Hirt (30) derived this condition by approximating the momentum equations with linear equations to which he applied a Fourier stability analysis. While both these criteria apply strictly only to Cartesian coordinates, the latter has been adequate for drop simulations in cylindrical coordinates.

The accuracy of the MAC method is difficult to predict because the error analysis of the method is significantly more complex than the method itself. The MAC manual (62) suggests qualitative guidelines for maintaining a reasonable degree of accuracy. The cell mesh should be fine enough that no variable changes by "much" across a cell width, and time steps should be short enough to prevent instability. However, worthwhile results can be obtained with the mesh made coarser than one might expect. Furthermore, the use of very fine spatial increments may backfire. Errors incurred when evaluating derivatives of field variables may be greatly magnified with fine grid spacing. Also fine spacing will require very small time increments in order to satisfy the condition (4.40). For example, decreasing δx to $\delta x/2$ will force δt to $\delta t/4$. The same considerations apply to the spacing of particles in the interface; a good "moderate" spacing should be selected by experiment. Since interior particles (noninterface) are used only for visualization, they require no special consideration.

CHAPTER 5. PROCEDURE

It was noted in Chapter 3 that the process of solving a transient fluid flow problem may be viewed as a suitable combination of a set of statements called the system with one or more functions called the input to produce one or more functions considered to be the output. The character of the system is governed by a set of quantities called parameters, and both input and output consist of variables which depend on position and time.¹

The numerical values of the parameters used in this study are listed in Table 5.1. They include purely physical properties, such as density and viscosity, descriptions of the initial condition, such as the initial drop volume, and quantities pertaining solely to the computation, such as the region and cell dimensions.

Figure 5.1 depicts the flow region, the initial drop profile, and part of the necessary computational apparatus. The flow region consisted of a mesh measuring 40 cells wide by 100 cells high, with each cell measuring 0.01 cm on each side. Cells were flagged according to their function and according to the type of fluid they contained. Interface particles were assigned to the interface curve at a regular interval of 0.005 cm, and about 400 free or internal particles were uniformly distributed inside the drop. In the interest of storage economy no particles were placed outside the drop.

¹These remarks may appear to belabor the obvious, but the formality is considered important here.

Table 5.1. Problem parameters

Parameter	Symbol	Value
PHYSICAL PROPERTIES		
Discontinuous fluid density	ρ_d	1.0 gm/cm ³
Continuous fluid density	ρ_c	0.6 gm/cm ³
Viscosity (both phases)	μ	2.0 cp
Interfacial tension	T_i	10.0 dynes/cm
Gravitation constant	g	980.662 cm/sec ²
NORMALIZED PROPERTIES ^a		
Viscosity	μ	6.3866×10^{-4} gm/cm ^{3/2}
Interfacial tension	T_i	1.0197×10^{-2} gm/cm
Gravitation constant	g	1.0
INITIAL CONDITIONS		
Bond number	Bo	0.430
Apex radius of curvature	R_o	0.1047 cm
Drop volume	V_o	9.457×10^{-3} cm ³
Interfacial area	A_o	0.2102 cm ²
GEOMETRICAL PROPERTIES		
Nozzle radius	R	8.0×10^{-2} cm
Width of fluid chamber	W	0.38 cm
Height of fluid chamber	H	0.98 cm
COMPUTATIONAL PARAMETERS		
Cell width	DX	1.0×10^{-2} cm
Interface particle spacing	DS	5.0×10^{-3} cm
Initial time increment (normalized)	DT	2.0×10^{-2} cm ^{1/2}
Region width	N_r	40 cells
Region height	N_z	100 cells

^a See Table 5.2.

Figure 5.1 also shows the types of boundary conditions used at the various fixed surfaces. Since the z-axis is a symmetry boundary the free-slip condition was used. In light of Sandry's (52) conclusion that a no-slip boundary condition works better at fixed surfaces in the vicinity of the nozzle than does a free-slip boundary condition, NOSLP cells were used at these surfaces. OUT cells were used at the

Figure 5.1. The flow region with the initial drop profile

upper and right-hand boundaries to approximate an infinite expanse of fluid. NOSLP cells were used at the base of the nozzle to represent a closed valve.

Initially, all velocities were set to zero, and pressures and the initial interface curve were established in the manner described in Chapter 4. The Bond number (based on the initial apex curvature) and the base radius were chosen to give a nonwetting drop possessing the critical volume. The difference between the densities of the two fluids was chosen much larger than in most physical systems, so that the larger buoyant forces would produce rapid accelerations, thereby causing the drop to separate more quickly. The chosen value of surface tension, while lower than typical, is at the threshold of the range of reasonable values. The value of viscosity is typical, and the value of g is the same as that used by Sandry (52).

With these conditions established, the drop hangs at rest in a tenuous state of equilibrium; the slightest upset will disturb the equilibrium and cause the drop to begin separating. Early attempts were made to induce flow through IN cells in the nozzle by manipulation of the nozzle pressure. While it was concluded that increasing the drop volume in this way (as in a laboratory experiment) would be the most realistic and achieve ultimate success, it was decided that this was too slow, and would produce a separation at the expense of excessive computer time. Instead, a gravity pulse equal to one additional g was applied long enough to accelerate a large portion of the drop, causing separation in a reasonably short time. This gravity pulse is somewhat analogous to shaking a drop off the tip of a pipet,

and formally constitutes the input to the system.

Jarring a drop loose in this way is not the usual reason for its detachment in an extraction column, but the separation it produces is a reasonably good approximation to the real event. It is concluded that, with the present level of development of the technique and available computing power, the gravity pulse perturbation would produce more results with lower expense.

Various exponents (9, 52) of the MAC method agree on the importance of smoothing the sequence of interface particles. However, some doubt has existed about how to smooth which particles, and when. Rather than try to apply some smoothness criterion, as did Daly (9), to discern which offending particle in the sequence is causing roughness, and then applying corrective measures, the author adopted the philosophy that it probably cannot be determined which particle or particles in a noisy sequence are causing the roughness. Instead all particles were regarded with suspicion, and a blanket smoothing was applied to the entire sequence at each time step. This was done for each particle by fitting a cubic to it and its ten nearest neighbors, and then replacing the particle coordinates by the coordinates of a point lying on the cubic. The second derivatives needed to compute curvature were then determined from the smoothed particle sequence and subjected to the same smoothing process.

During the course of the simulation the size of the time increment was automatically adjusted at each time frame according to the maximum velocity in the region, so that no fluid element would ever travel more than one third of a cell width during one time step. Consequently,

successive frames each showed about the same amount of information.

In a computational problem of this type it is often advantageous to express variables in a dimensionless or reduced form. The reduced solution may then be applied to various situations by scaling the variables. Dimensional analysis of the Navier-Stokes equation (2, p. 107) shows that it is characterized by two dimensionless groups. They are the Reynolds number,

$$Re = \rho v d / \mu$$

and the Froude number,

$$Fr = v^2 / dg$$

The Reynolds number represents the ratio of inertial forces to viscous forces, while the Froude number represents the ratio of inertial forces to gravitational forces. If two systems possess the same Reynolds and Froude numbers, and the same initial and boundary conditions, then they are dynamically similar.

Unfortunately, both groups contain a velocity, making their definition awkward in the solution of an initially quiescent system. Consequently a normalizing system used by Sandry (52) was adopted. In this scheme the momentum equation is normalized by division by g . Time is replaced by $tg^{1/2}$ and velocity by $\bar{U}/g^{1/2}$. The variables and parameters which assume normalized forms are listed in Table 5.2.

The application of the gravity pulse establishes, at the start of the simulation, an imbalance of body forces and surface tension forces. The net force on the drop causes the major portion of it to

Table 5.2. Normalized variables

Name	Symbol	Normalized form
Gravitation constant	g	1
Time	t	$tg^{1/2}$
Velocity	u, v	$ug^{1/2}, vg^{1/2}$
Pressure	p	p/g
Viscosity	μ	$\mu/g^{1/2}$
Interfacial tension	T_i	T_i/g

deform and extend in the direction of the gravitation vector. Each of the resulting successive profiles is mechanically unstable, and the bulk of the drop continues to accelerate. As the profile becomes distended, continuity requires the neck to narrow. The surrounding medium flows out of the way of the apex of the drop, and into the region voided by the neck.

The process continues until the neck is so narrow that detachment is imminent. A finite difference calculation lacks the resolution needed to compute, at the molecular level, the topological transformations accompanying detachment. Therefore, the computation must be terminated at some time, and the results used to construct the initial conditions of a sequel, which is the simulation of the post-detachment flow. No method is yet known for determining exactly when detachment should occur, and the decision is essentially a matter of judgment. In this work detachment was accomplished when the interface approached the centerline to within $DX/2$ by instructing the simulation program to

treat the interface sequence as two distinct sequences. The rough edges formed by this division were smoothed by an application of the smoothing algorithm to each sequence.

CHAPTER 6. RESULTS

Enumeration of Results

A useful characteristic of the type of output obtained from the drop flow simulation program is that the data are easily represented in pictorial fashion for visual analysis. The primary output consists of two files, one containing a time sequence of snapshots of particle positions, the other a series of views of the velocity field. Computer-generated plots of these files greatly facilitate interpretation of the course taken by the simulation.

Figures 6.1 through 6.4 show a complete set of successive interface curves, from the initial profile, through elongation, detachment, and departure of the separated drop. Comparison of these curves with examples of experimental profiles shows that the simulation has successfully exhibited nearly all of the expected topological transformations, the only notable exception being the failure to produce a satellite droplet.

Figures 6.5 and 6.6 show successive profiles from $T = 0.0$ to impending detachment, and show the locations of internal particles. These views are of great value in illustrating the strain experienced by the internal fluid, especially near the interface. Plots of internal particles after separation are not included because of an unfortunate tendency of particles to "tunnel" across the interface and into the surrounding medium. The exact cause of this problem is uncertain, but may be due to a possible oversmoothing of the interface particles during the detachment period, when time increments are very short

Figure 6.1. Successive profiles at $T = 0.0, 0.5, 1.0$, and 1.3

Figure 6.2. Successive profiles at $T = 1.5, 1.6, 1.7,$ and 1.781

Figure 6.3. Successive profiles at $T = 1.782, 1.80,$ and 1.82

Figure 6.4. Successive profiles at $T = 1.84, 1.86,$ and 1.88

Figure 6.5. Successive profiles at $T = 0.0, 1.0$, and 1.5 , showing the locations of internal particles

Figure 6.6. Successive profiles at $T = 1.7$ and 1.781 , showing the locations of internal particles

and the smoothing algorithm is applied at a high frequency.

Figures 6.7, 6.8, and 6.9 show a sequence of profiles on which are superimposed representations of the velocity fields. Each arrow represents the magnitude and direction of the local velocity at the tail of the arrow. To facilitate clear representation of a wide range of velocities, the lengths of the arrows were logarithmically scaled to the velocity magnitudes by the rule

$$L = (SF)L_{\max}$$

where L is the length in plot axis centimeters, $L_{\max}$ is the maximum possible length, and SF is a scale factor. The latter is calculated according to

$$SF = \log(V/V_{\min}) / \log(V_{\max}/V_{\min})$$

in which V is the magnitude of the local velocity, $V_{\min}$ is the lowest magnitude to be represented, and $V_{\max}$ is the largest magnitude that will ever occur. In the simulation this peak velocity was numerically equal to $2.127 \text{ cm}^{1/2}$, and occurred during detachment ($T = 1.7810 \text{ cm}^{1/2}$) at the point of detachment. The value of $V_{\min}$ was chosen to be exactly $0.001 V_{\max}$, allowing representation of three orders of magnitude. Any magnitude less than $V_{\min}$ would cause an arrow of negative length to be drawn, and was suppressed. A magnitude of $V_{\max}$ would cause an arrow of length $L_{\max}$ to be drawn. Arrows were drawn at intervals of 0.08 cm , and $L_{\max}$ was chosen to be exactly half of this.

Figures 6.7 through 6.9 show rather strikingly the formation of a vortex tube around the widest portion of the drop. Not surprisingly,

Figure 6.7. Eulerian velocity plots at $T = 0.5, 1.0, 1.3$, and 1.5

Figure 6.8. Eulerian velocity plots at $T = 1.6, 1.7, 1.781$, and 1.782

Figure 6.9. Eulerian velocity plots at $T = 1.80, 1.84$, and 1.88

the vortex follows the drop up the z-axis, until the termination of the run.

Whereas the preceding discussion concerned velocities viewed in the Eulerian sense i.e., from a fixed frame of reference, Figures 6.10 and 6.11 depict velocities in the Lagrangian sense. The velocities are those seen by an observer moving with the drop and are computed by subtracting the magnitude of the apex velocity, v_a , from the vertical component of local velocity. The apex velocity may be taken as a measure of the average velocity of the separating portion of the drop. These plots demonstrate a variation of the vortex phenomenon discussed above: a vortex exists inside the drop. This is an interesting adjunct to the conclusion of Garner and Skelland (16), who attributed internal circulation to flow through the nozzle. No liquid flows through the nozzle in this simulation.

These Lagrangian velocity plots, and their details in Figures 6.12 and 6.13, show that the flow is similar to the classic solution for flow past a sphere, as described by Happel and Brenner (23, p. 127). An important difference is in the existence of the peculiar post-detachment wake between the separated drop and the collapsing neck.

To complete the representation of velocities Figures 6.14 and 6.15 show Eulerian details of the collapse of the neck into the base after detachment. These diagrams serve to illustrate the power of the computational approach in studying an extremely rapid event. High speed motion picture studies of actual separations, such as that in Figure 1.1 may not be fast enough to resolve the collapse of the neck, which may occur between two successive frames. The last three frames

Figure 6.10. Lagrangian velocity plots at $T = 1.0, 1.5, 1.7$, and 1.781 . These are velocities relative to the motion of the apex

Figure 6.11. Lagrangian velocity plots at $T = 1.782$, 1.80, 1.84, and 1.88

Figure 6.12. Detail Lagrangian velocity plots at $T = 1.0, 1.5, 1.7,$ and 1.781

Figure 6.13. Detail Lagrangian velocity plots at $T = 1.782, 1.80, 1.84$, and 1.88

Figure 6.14. Detail of the collapse of the neck into the base. $T = 1.782, 1.80, 1.82, \text{ and } 1.84$.

Figure 6.15. Detail of the collapse of the neck into the base. $T = 1.86$ and 1.88

in Figure 1.1 are spaced 2.5 ms apart, while the time increment in the simulation was as short as 40 μ s at detachment.

Figures 6.16 and 6.17 illustrate the cause/effect relationship of input or forcing function to the system response. Figure 6.16 shows the gravity pulse and the variation of the maximum velocity with time. The maximum velocity is always located on the z-axis in the neck region. It was noted previously that its peak value occurs at the instance of detachment in both time and position. The small peak in the maximum velocity curve at $T = 0.25$ is absent in the plot of the vertical component, showing that it is purely a variation in the horizontal component. The reason for the fluctuation is not yet known, but is believed to be a numerical disturbance associated with the time increment scaling process used in the program. The small peak occurring after separation is attributed to a true physical post-detachment oscillation.

The top half of Figure 6.17 shows the corresponding time response of the apex velocity. The scatter of points about the smoothed curve is attributed to numerical variations of velocities in the interface cells. The dip in the curve after oscillation is likely due to an expected physical oscillation.

The bottom half of Figure 6.17 contains a plot of the variation of total drop volume and a dimensionless surface-to-volume ratio. The variation of drop volume is a measure of the violation of the continuity equation, and shows a total volume conservation error of only about 8%. The plot of the surface-to-volume ratio indicates that the deformation occurring before detachment tends to force the liquid away from a minimum-area condition, but after the climax of

Figure 6.16. Maximum velocity curves and the gravitation pulse

Figure 6.17. Apex velocity, total drop volume, and surface-to-volume ratio curves. The curves in the lower portion are plots of normalized data, obtained by dividing each value by the initial value (See Table 5.1.)

detachment interfacial tension tends to restore the minimum-area condition. The small blips in each curve at detachment are due to volume conservation errors associated with artificially reconfiguring the interface curve.

Table 6.1 contains a list of miscellaneous results. Although the difficulty of defining a Reynolds number was noted earlier, a "separation Reynolds number" has been included. This value is based on the apex velocity and drop diameter (both measured at detachment), and on the density of the surrounding fluid. A terminal velocity, computed by Stokes law for a freely descending sphere, and its associated Reynolds number are included for comparison.

Table 6.1. Results

Quantity	Symbol	Normalized value	Unnormalized value
Time to separation	t_s	$1.781 \text{ cm}^{1/2}$	56.9 ms
Neck velocity at separation	v_{ns}	$2.127 \text{ cm}^{1/2}$	66.6 cm/s
Apex velocity at separation	v_{as}	$0.225 \text{ cm}^{1/2}$	7.05 cm/s
Separation Reynolds number ^a	Re_s	53.5	
Separated drop radius	r_d	0.1255 cm	
Theoretical terminal velocity	v_t	$2.23 \text{ cm}^{1/2}$	69.8 cm/s
Theoretical Reynolds number ^b at terminal velocity	Re_t	530	

$$^a Re_s = 2\rho_c v_{as} r_d / \mu.$$

$$^b Re_t = 2\rho_c v_t r_d / \mu.$$

Comparison to Experimental Results

Attempts to make a detailed comparison of the results of the simulation with results obtained in the laboratory are hampered by the unavailability of data on a physical system whose parameters are equal to those in Table 5.1. Accuracy of the results may, however, be assessed on a qualitative or order-of-magnitude scale.

A preliminary judgment of the general correctness of the simulation may be made by comparing the successive simulated profiles with those from experiment. For example, the profile of the water drop in Figure 1.1 undergoes essentially the same transformations as does the simulation profile. Since these profiles are functions of velocity, which is interrelated with pressure, confidence is bestowed on the validity of the computed velocities and pressures.

Seemann (57) experimentally measured velocities along the centerline of a drop of cyclohexane separating in water. His measurements at several instants immediately before separation show velocity rising slightly from the apex velocity, remaining constant down the bulk of the separating portion, rising to an extreme peak in the neck, and tapering to zero toward the base. The region between the apex and the neck is almost in a state of plug flow; the relationship between its velocity and that of the apex is evidence of the existence of a circulation pattern similar to that in Figures 6.12 and 6.13. For a drop whose separated radius was about 0.7 cm the apex velocity at detachment was about 9 cm/s. The neck velocity was too large to measure, but at 0.01 seconds before detachment was estimated at about

35 cm/s. By extrapolation, the neck velocity appears to be about double that value at detachment.¹ The apex and neck velocities (7.05 cm/s and 66.6 cm/s) of the simulated drop therefore appear to be reasonable.

¹This, of course, is only an estimate and is based on the motions of tracer particles observed in the neck region in the moments before detachment. The peak neck velocity at detachment, determined in the simulation, is actually an average for the cell in which detachment occurs. Since the detachment transformation takes place at the molecular level, its true value is largely indeterminate, and may even approach molecular velocities.

CHAPTER 7. EPILOGUE

Evaluation

The significance of this study, and its results, should be established by inquiring what it has contributed to the body of knowledge of drop phenomena. Tantamount to this is to ask what it has shown that previous investigations have failed to do. These questions may be answered by returning to the older computations discussed in Chapter 2.

Primarily, the outcome of this study clearly shows, where the computational model of Sandry (52) did not, that a complete drop separation can be simulated by numerical solution of the full momentum equations. Moreover, in comparison to the more rudimentary computations of Halligan and Burkhart (19), Seemann (57), and others (29, 47, 53), the success of this experiment is evidence that proper solution of the complete equations is the minimum effort required to obtain reliable solutions.

It is not this author's intent to present the numerical results as new and hitherto unknown. Many of the same information may be, and in some cases has been, obtained through shrewd laboratory investigations. Rather, it is hoped that this simulation will provide the laboratorian a much needed fresh view of the phenomenon which he has had to study by careful interpretation of his own observations. Haugering (22) has eloquently declared,

"The purpose of computing is insight, not numbers."

This author's philosophy is in perfect conformity with that observation. The belief that computational insight should supplement experimental insight is paramount; it is hoped that the junction of both avenues of inquiry will lead to a higher stage of understanding than either could produce independently.

An excellent example is the study of the velocity field both inside and outside the drop. Experimentalists such as Seemann (57) have been able to measure, by tedious means, velocities at discrete points, provided such velocities are not too extreme. Considerable interpretation is required to convert these measurements into overall flow patterns. The simulation, on the other hand, reveals these patterns at a glance.

The overall success of this venture should be measured against its goals, and against its difficulty. The primary goal has been to construct a model which expresses in mathematical terms the relationships which are observed in physical experience, or are inferred from observations. Evaluation of the results, and comparison to laboratory experiments, demonstrates that a high degree of success has been achieved.

Certainly the most difficult part of the work was the development of an implementation of the interface boundary condition suitable for unsteady state flow calculations. Previous attempts to broach this problem have been discussed in Chapters 2 and 3; they proved inadequate either because they were incomplete, or because they dealt with values of parameters (specifically surface tension) which were outside the range of interest. An essential goal has been to mold the constituent

elements of earlier methods, together with necessary specific refinements, into a single coherent, easily applied procedure. In this respect the effort is deemed largely successful.

At the outset much uncertainty existed whether a computational attack on the drop flow problem was even feasible. It remained to be answered not whether we can compute the flows, but whether we can, with a reasonable amount of effort, construct a program to direct a general purpose digital computer to an accurate solution, without placing unreasonable demands on computing resources. During the time of the evolution of the MAC method one of the few places which possessed the necessary resources, and at which this type of calculation could even be considered, was Los Alamos itself. The MAC method was developed with the aid of the Los Alamos STRETCH computer which was designed to perform high-speed calculations on large arrays. With considerable amounts of main storage at their disposal, the group there could afford to employ very simple, albeit inefficient, expedients in order to handle the overhead associated with conducting a simulation. An excellent case-in-point is their method of estimating cellular densities which, although fast, makes rather extravagant use of storage.

Obviously, the design of a program of this complexity involves compromises, with the trade-offs usually being efficiency of execution against use of random-access memory. To be considered as a suitable vehicle for performing unsteady state flow calculations, a computing system must provide copious amounts of both computing power and storage. The system at the Iowa State University Computation Center, while easily satisfying both requirements, made it desirable to opt for

less storage utilization than for higher execution efficiency. In the example of the previous paragraph, the cell density calculation was replaced with one requiring considerably less storage, but involving many routine operations.

Inasmuch as compromise is an essential ingredient in the design of a complex simulation model, it is understood that approximations are part of its construction. These approximations are naturally manifest as deviations in the results. This truth is certainly apparent in the present study.

One might wonder what is the value of a model riddled with approximations. Hamming (Burkhart, 4) has also stated,

"What we need are fewer exact solutions to approximate problems and more approximate solutions to exact problems."

This notion represents a turning from the strategy of early investigators, whose best hope was to condense a complex insoluble problem into a simpler form which they could solve analytically. Unfortunately, there has often been a strong temptation to place uncritical faith in the consequent solution which, although beautiful and concise, has only limited bearing on the real situation. Early studies, therefore, were committed at the outset to approximations, while later studies were limited in accuracy only by existing levels of computing ability. As computing methods improve, approximate solutions of exact problems tend toward truth itself.

Conclusions

The primary conclusion of this study is that it is feasible to construct a model of drop flow behavior with results obtained by numerical solution of the momentum and continuity equations. The effort has produced a model which shows stable and realistic behavior well past separation, a feat not even approached by earlier models.

It is concluded that a two-phase calculation of the flows is necessary, while a single-phase calculation is inadequate. It is further concluded that the assumptions and approximations used in expressing computational forms of the continuum equations, and the model of the interface used to construct the interface boundary condition are adequate. It is not concluded that the approach to smoothing the interface particle sequences is necessarily the most accurate, the most reliable, or the most efficient. However, significant ground has been covered on this problem, and a simple process of fine-tuning may be enough to produce the necessary economy and precision needed to apply the smoother to a series of production calculations.

Recommendations for Future Studies

With the developmental burden out of the way it is recommended that effort now be devoted to a program of tests to evaluate the accuracy of the model. Experiments with various types of perturbations should be attempted. Tests should be performed to determine an optimum bandwidth for the interface smoother.

This study has employed a highly simplified model of the interface, incorporating only its curvature and equilibrium interfacial tension. Scriven (55, 56) has systematized the rheological behavior of a Newtonian fluid interface, which is characterized by both interfacial tension and surface viscosity. It may be possible to adapt his analysis to a refinement of the interface boundary condition.

On a larger time scale, the model should eventually be applied to the purpose for which it was originally intended: lending insight into the elemental nature of heat and mass transfer during drop formation and separation.

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ACKNOWLEDGMENTS

Much credit is due to Dr. Lawrence E. Burkhart for his overall guidance and helpful criticism during this study, and for his contagious enthusiasm. Thanks are also given to Dr. Thomas D. Sandry for many hours of consultation, and for establishing the background for this project. The author acknowledges the assistance of the entire staff of the Iowa State University Computation Center, particularly Mr. William S. Frazier, Jr. The author also acknowledges Dr. Richard C. Hoyt for much informal discussion, and Mr. James A. Herriott for assistance in the laboratory. The author credits the patience and skill of Letha Osmundson, who typed the manuscript. Finally, the author owes much to his parents for making graduate study possible, and to his wife, Judy, whose patience and understanding are immeasurable.

APPENDIX.

EXPANSION OF THE VECTOR CONTINUUM

EQUATIONS IN CYLINDRICAL COORDINATES

This appendix provides material supplemental to the algebraic manipulations of Chapter 3, and specifically contains cylindrical coordinates expansions of the incompressibility, momentum, and pressure equation. References for the discussion are McConnell (43), Appendix A in Bird, Stewart, and Lightfoot (2), Menzel (44), and Korn and Korn (35).

Cylindrical Coordinates

The reciprocal transformation equations for Cartesian coordinates (x, y, z) and cylindrical coordinates (r, θ, z) are

$$\begin{aligned}x &= r \cos \theta \\y &= r \sin \theta \\z &= z\end{aligned}\tag{A.1}$$

and

$$\begin{aligned}r &= (x^2 + y^2)^{1/2} \\\theta &= \tan^{-1}(y/x) \\z &= z\end{aligned}\tag{A.2}$$

That the cylindrical coordinate system is orthogonal may easily be verified by transforming the components of the metric tensor in Cartesian coordinates, namely

$$g_{pq} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

where p and q index x, y, and z, into cylindrical coordinates to produce

$$\begin{aligned} \bar{g}_{ij} &= \frac{\partial x^p}{\partial \bar{x}^i} \frac{\partial x^q}{\partial \bar{x}^j} g_{pq} \\ &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned} \quad (\text{A.3})$$

in which x^p represents x, y, or z, and $\bar{x}^i$ represents r, θ , or z.¹ Since the off-diagonal elements of $\bar{g}_{ij}$ are zero the coordinate system is orthogonal. In addition the associated metric tensor is the inverse, namely

$$g^{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/r^2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (\text{A.4})$$

and the scale factors are

¹In contrast to the notation of Chapters 3 and 4, an overbar ($\bar{A}$) is used here to represent a transformed quantity, a single underscore ($\underline{A}$) represents a vector, and a double underscore ($\underline{\underline{A}}$) represents a second-order tensor. For example, the transformed and untransformed covariant components of the tensor $\underline{\underline{A}}$ may be written in the equation

$$\underline{\underline{A}} = \underline{e}_i \underline{e}_j A^{ij} = \underline{e}_k \underline{e}_l \bar{A}^{kl}$$

The summation convention for umbral indices is used throughout this appendix.

$$\begin{aligned}
 h_1 &= \sqrt{g_{11}} = \sqrt{1} = 1 \\
 h_2 &= \sqrt{g_{22}} = \sqrt{r^2} = r \\
 h_3 &= \sqrt{g_{33}} = \sqrt{1} = 1
 \end{aligned}
 \tag{A.5}$$

Equation of Incompressibility

The general continuity equation may be written

$$\frac{D\rho}{Dt} = -\rho(\underline{\nabla} \cdot \underline{U}) \tag{A.6}$$

or

$$\frac{\partial \rho}{\partial t} + (\underline{U} \cdot \underline{\nabla})\rho = -\rho(\underline{\nabla} \cdot \underline{U}) \tag{A.7}$$

and expresses total mass conservation. By setting density, ρ , constant we obtain the equation of incompressibility,

$$\underline{\nabla} \cdot \underline{U} = 0 \tag{A.8}$$

which expresses volume conservation. However Equation (A.8) may be used as the starting point rather than

$$\rho = \text{constant} \tag{A.9}$$

Substituting (A.8) into (A.7) yields

$$\frac{\partial \rho}{\partial t} + (\underline{U} \cdot \underline{\nabla})\rho = 0 \tag{A.10}$$

This result expresses that changes in local density viewed by a fixed observer are due only to the motion of an incompressible fluid of possibly variable density. It is seen that Equation (A.9) is much

more restrictive than (A.8). This important difference is an essential part of the two-fluid form of the MAC method.

The quantity $\nabla \cdot \underline{U}$, denoted by D , is the divergence of the velocity, and is sometimes called the discrepancy or dilation by various authors. The derivative may be formed in any coordinate system by taking the covariant derivative $\nabla \underline{U}$, and contracting to form the inner product. Bird, Stewart, and Lightfoot (2) give the expansions of several differential operations involving vectors and tensors in rectangular, cylindrical, and spherical coordinates. In cylindrical coordinates,

$$\nabla \cdot \underline{U} = \frac{1}{r} \frac{\partial}{\partial r} (ru_r) + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{\partial u_z}{\partial z} \quad (\text{A.11})$$

For two-dimensional flows in which azimuthal components of velocity and gradient vanish, the equation of incompressibility becomes

$$\frac{1}{r} \frac{\partial}{\partial r} (ru) + \frac{\partial v}{\partial z} = 0$$

where u and v denote the r and z components of $\underline{U}$.

Momentum Equation

The momentum equation may be written in terms of variable density and viscosity in the form

$$\begin{aligned} \frac{\partial(\rho \underline{U})}{\partial t} = & - \nabla \cdot (\rho \underline{U} \underline{U}) - \nabla p \\ & + 2(\nabla \cdot \underline{\mu} \underline{\nabla}) \underline{U} + \nabla X(\underline{\mu} \underline{\nabla} X \underline{U}) + \rho \underline{g} \end{aligned} \quad (\text{A.12})$$

Bird, Stewart, and Lightfoot (2) provide expansions in cylindrical coordinates for all except the viscous terms. Since the derivative

of a vector equals the sum of the derivatives of its components the time derivative becomes

$$\frac{\partial(\rho \underline{U})}{\partial t} = \underline{e}_r u_r + \underline{e}_\theta u_\theta + \underline{e}_z u_z \quad (\text{A.13})$$

in which $\underline{e}_r$, $\underline{e}_\theta$, and $\underline{e}_z$ are the unit vectors. Consequently Equation (A.12) should be expressed as three scalar equations for three velocity components. Since only the r and z components of velocity and gradient are used in this study, all θ components may be eliminated beforehand. Thus Equation (A.13) reduces to

$$\frac{\partial(\rho \underline{U})}{\partial t} = \underline{e}_r u + \underline{e}_z v \quad (\text{A.14})$$

The convective term in Equation (A.12) is the divergence of $\rho \underline{U} \underline{U}$, a symmetrical tensor. From the reference the r and z components are

$$\begin{aligned} (\nabla \cdot \rho \underline{U} \underline{U})_r &= \frac{1}{r} \frac{\partial}{\partial r} (ru^2) + \frac{\partial}{\partial z} (uv) \\ (\nabla \cdot \rho \underline{U} \underline{U})_z &= \frac{1}{r} \frac{\partial}{\partial r} (ruv) + \frac{\partial}{\partial z} (v^2) \end{aligned} \quad (\text{A.15})$$

The pressure gradient is just the gradient of a scalar quantity and is

$$\underline{\nabla} p = \underline{e}_r \frac{\partial p}{\partial r} + \underline{e}_z \frac{\partial p}{\partial z} \quad (\text{A.16})$$

Also the body force term is expressed

$$\rho \underline{g} = \underline{e}_r \rho g_r + \underline{e}_z \rho g_z \quad (\text{A.17})$$

The forms for the two viscous terms are not given by Bird, Stewart, and Lightfoot (2) but may be derived using formal tensor calculus. To evaluate the first term we make use of the identity

$$(\nabla \cdot \mu \nabla) \underline{U} = \nabla \cdot [\mu (\nabla \underline{U})] \quad (\text{A.18})$$

Expressing $\underline{U}$ in terms of its contravariant components,

$$\underline{U} = \underline{e}_i u^i$$

in which $\underline{e}_i$ are the covariant unitary base vectors. The first differentiation produces the tensor

$$\begin{aligned} \nabla \underline{U} &= \nabla (\underline{e}_i u^i) \\ &= \underline{e}^j \underline{e}_i u^i_{\cdot,j} \\ &= \underline{e}^j \underline{e}_i A^i_{\cdot,j} \\ &= \underline{\underline{A}} \end{aligned} \quad (\text{A.19})$$

in which $u^i_{\cdot,j}$ are the components of the covariant derivative of $\underline{U}$ and $A^i_{\cdot,j}$ are the mixed components of $\underline{\underline{A}}$. Multiplying by the scalar μ gives

$$\begin{aligned} \underline{\underline{B}} &= \mu \underline{\underline{A}} \\ &= \mu (\underline{e}^j \underline{e}_i A^i_{\cdot,j}) \\ &= \underline{e}^j \underline{e}_i (\mu A^i_{\cdot,j}) \\ &= \underline{e}^j \underline{e}_i B^i_{\cdot,j} \end{aligned} \quad (\text{A.20})$$

Before forming and contracting the second derivative the index j must be raised in (A.20) as follows:

$$\begin{aligned}
\underline{\underline{B}} &= (\underline{e}_k g^{jk}) \underline{e}_i B^i_{.j} \\
&= \underline{e}_k \underline{e}_i (g^{jk} B^i_{.j}) \\
&= \underline{e}_k \underline{e}_i B^{ik} \\
&= \underline{e}_j \underline{e}_i B^{ij}
\end{aligned} \tag{A.21}$$

The divergence of this is the contracted covariant derivative,

$$\underline{\nabla} \cdot \underline{\underline{B}} = \underline{e}_i B^{ij}_{\dots,j} \tag{A.22}$$

When the indicated algebra is performed the final result, in terms of physical vector components, is

$$\begin{aligned}
[(\underline{\nabla} \cdot \mu \underline{\nabla}) \underline{U}]_r &= \frac{1}{r} \frac{\partial}{\partial r} (r \mu \frac{\partial u_r}{\partial r}) + \frac{1}{r^2} \frac{\partial}{\partial \theta} [\mu (\frac{\partial u_r}{\partial \theta} - u_\theta)] \\
&\quad + \frac{\partial}{\partial z} (\mu \frac{\partial u_r}{\partial z}) - \frac{\mu}{r^2} (\frac{\partial u_\theta}{\partial \theta} + u_r) \\
[(\underline{\nabla} \cdot \mu \underline{\nabla}) \underline{U}]_\theta &= \frac{\partial}{\partial r} [\mu (r \frac{\partial}{\partial r} (\frac{u_\theta}{r}) + \frac{u_\theta}{r})] + \frac{1}{r^2} \frac{\partial}{\partial \theta} [\mu (\frac{\partial u_\theta}{\partial \theta} + u_r)] \\
&\quad + \frac{\partial}{\partial z} (\mu \frac{\partial u_\theta}{\partial z}) \\
[(\underline{\nabla} \cdot \mu \underline{\nabla}) \underline{U}]_z &= \frac{1}{r} \frac{\partial}{\partial r} (r \mu \frac{\partial u_z}{\partial r}) + \frac{1}{r^2} \frac{\partial}{\partial \theta} (\mu \frac{\partial u_z}{\partial \theta}) + \frac{\partial}{\partial z} (\mu \frac{\partial u_z}{\partial z})
\end{aligned} \tag{A.23}$$

These are the components of one-half the first viscous term.

The second viscous term requires two repeated curl operations, as seen by writing it as $\underline{\nabla} \times [\mu (\underline{\nabla} \times \underline{U})]$. The first differentiation may be expressed

$$\begin{aligned}
\underline{\nabla} \times \underline{U} &= \underline{\nabla} \times (\underline{e}^i u_i) \\
&= (\underline{e}^j \times \underline{e}^i) u_{i,j}
\end{aligned}$$

$$= \underline{e}_k \epsilon^{jik} u_{i,j} \quad (\text{A.24})$$

in which ϵ^{jik} are the contravariant components of the permutation tensor and take the values

$$\begin{aligned} \epsilon^{123} &= \epsilon^{231} = \epsilon^{312} = 1/\sqrt{g} \\ \epsilon^{321} &= \epsilon^{213} = \epsilon^{132} = -1/\sqrt{g} \\ \epsilon^{iij} &= \epsilon^{iji} = \epsilon^{iij} = 0 \end{aligned}$$

Multiplying (A.24) by μ ,

$$\begin{aligned} \mu (\nabla \times \underline{U}) &= \mu (\underline{e}_k \epsilon^{jik} u_{i,j}) \\ &= \underline{e}_k A^k \end{aligned}$$

and lowering the index k ,

$$\begin{aligned} \mu (\nabla \times \underline{U}) &= (\underline{e}^k g_{sk}) A^k \\ &= \underline{e}^s (g_{sk} A^k) \\ &= \underline{e}^s A_s \\ &= \underline{e}^k A_k \end{aligned} \quad (\text{A.25})$$

Forming the second curl,

$$\begin{aligned} \nabla \times [\mu (\nabla \times \underline{U})] &= \nabla \times (\underline{e}^k A_k) \\ &= (\underline{e}^1 \times \underline{e}^k) A_{k,1} \\ &= \underline{e}_m \epsilon^{1km} A_{k,1} \\ &= \underline{e}_m B^m \end{aligned} \quad (\text{A.26})$$