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Improved Free Surface Boundary Conditions for Numerical Incompressible-Flow Calculations*

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Complete free surface stress conditions have been incorporated into a numerical technique for computing transient, incompressible fluid flows. An easy to apply scheme, based on a new surface pressure interpolation, permits the normal stress to be applied at the correct free surface location. Tangential stresses are applied through the assignment of appropriate velocities near the surface. To illustrate the influence of the complete stress conditions, a variety of examples are presented, including some with highly contorting and colliding surfaces. Several of the examples are compared with experimental and analytical results. The influence of these boundary conditions on numerical stability is discussed from a simple qualitative point of view.

INTRODUCTION

Improvement of the free surface boundary conditions used in numerical fluid flow calculations is a continuing need. The Marker-and-Cell (MAC) method [1] has been significantly improved in this area by several recent investigators. The basis of these improvements has been in satisfying the free surface stress conditions more accurately. Crude approximations to these conditions were used in the original marker-and-cell method. Later, better approximations to the normal stress conditions were incorporated by Hirt and Shannon [2]. At that time, however, all pressures were specified at the calculational cell centers; therefore, while the correct normal stress was calculated it was not always applied at the correct location of the surface. It was then pointed out by Chan *et al.* [3] that the pressure could be specified at the surface instead of the nearby cell center by use of variable space increments. They devised a better finite-difference approximation to the Poisson equation for pressure that is applicable to many free surface problems for inviscid fluids.

Both of these previous improvements have now been utilized to apply the correct normal and tangential stress conditions to the exact fluid surface location. To accomplish this a pressure interpolation technique has been developed, which,

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due to its logical simplicity, can be easily incorporated into existing MAC method computer codes. Another advantage of this scheme is that it retains one of the main advantages of the Eulerian computational methods, i.e., the ability to calculate highly contorted, colliding surfaces [4]. This scheme is herein described in detail. The tangential stress condition has not, to our knowledge, previously been incorporated in numerical techniques. In this paper we also discuss when these conditions should be included, and the influence they have on numerical stability. To illustrate the influence of the complete stress conditions a variety of examples are presented and compared with both experimental and analytical results.

The Marker-and-Cell Method

The marker-and-cell method was designed to calculate the flow of a viscous, incompressible fluid having a free surface [1]. Complete details of this method and numerous calculational examples can be found in the cited references; however, a brief description of the technique is given here of those features needed to understand this paper.

The MAC method employs an Eulerian mesh of calculational cells and finite difference expressions to approximate the equation of continuity and the Navier–Stokes equations. The primary dependent variables are the pressure and the velocity components of the fluid. The pressure is specified at the center of each Eulerian cell and is determined through the solution of a Poisson equation for pressure. A staggered mesh is used in the velocity component placement, which specifies the normal velocities at the Eulerian cell boundaries (see Fig. 1).

The distinguishing feature of the MAC method is its capability to calculate free surface flows. The fluid surface is delineated by marker particles that move through the stationary network of cells. Each Eulerian cell is flagged to denote whether it is an empty cell (E) containing no fluid, a surface cell (S), which contains fluid but is next to an empty cell, or a full cell (F), which contains fluid and is not next to an empty cell. An example of this labeling is shown in Fig. 1. The purpose of this paper is to give prescriptions for the assignment of velocities and pressures in surface (S) cells that insure the satisfaction of the complete free surface stress conditions.

The Normal Stress Condition

The normal and tangential stress conditions for a two-dimensional surface can be approximated by the expressions [2]

$$\phi - 2\nu(\partial u_n/\partial n) = 0, \tag{1}$$

$$\nu(\partial u_n/\partial m + \partial u_m/\partial n) = 0, \tag{2}$$

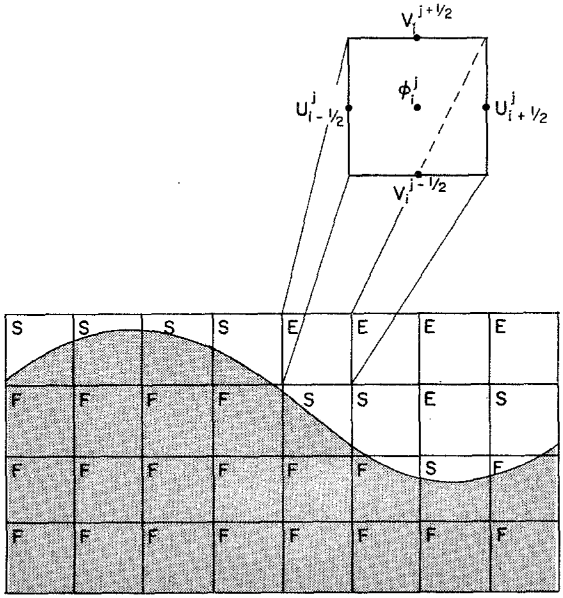

FIG. 1. Field-variable layout and cell flags.

where n denotes the outward normal direction and m the tangential direction to the local free surface; ϕ refers to the ratio of pressure to constant density, u_n is the normal and u_m the tangential velocity, and ν the kinematic viscosity of the fluid. Expressions (1) and (2) are to be applied at the surface.

Originally the normal stress condition in MAC was approximated by setting the pressure equal to zero in all surface cells. Later [2] the surface cell pressure was modified to include the normal viscous stress according to (1). This pressure was still specified at the cell center, however, regardless of the location of the surface within the cell. The correct application of the normal stress condition necessitates the determination of both the surface slope and location within the surface cell.

The surface slope can be determined approximately through the use of the cell flagging scheme. For example, if the cell above the surface cell is the only adjacent empty cell, then the surface is considered to be horizontal; if both the cell to the left and the one above the surface cell are empty, then the surface is considered to be oriented 45° to the horizontal. A more exact slope could be determined, but we have found this simple approximation to be adequate. The appropriate normal stress, which depends on the slope, is then derived from Eq. (1). A complete discussion of this is given in Ref. [2].

In contrast to Ref. [2], however, this pressure is now applied at the actual fluid surface. To accomplish this, a pressure at the center of the surface cell is specified as a linear interpolation (or extrapolation) between an adjacent full cell pressure and the desired pressure at the fluid surface. Before writing down the interpolation formula, however, we must first define what is meant by the surface position within a calculational cell.

The surface is specified by a set of marker particles that move with the local fluid velocity. The surface is defined by the line segments connecting these points in sequential order.

A proper cell center pressure is calculated in terms of an interpolation factor, $\eta = \delta y/d$, where d is the distance from the actual surface to the center of a neighboring full cell along a line connecting the surface cell and full cell centers. To calculate d the sequentially numbered surface markers on either side of the line connecting cell centers is determined. The point of intersection of a line segment between these bracketing surface markers and the line connecting cell centers is determined. The distance between this point and the center of the adjacent full cell is d, as shown in Fig. 2. Similar distances are calculated for all full cells adjacent to

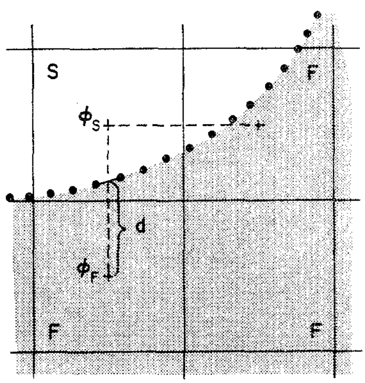

FIG. 2. A typical interpolation cell selection.

the surface cell. When there is more than one neighboring full cell, the one having the smallest value of $|\delta y - d|$ or $|\delta x - d|$ is chosen for the interpolation. This is the cell whose intersection point is nearest the center of the surface cell. The pressure in the surface cell is then calculated by a linear interpolation

$$\phi_s = \eta(\phi_a + \phi_{ns}) + (1 - \eta)\,\phi_f\,, \tag{3}$$

where ϕ_{ns} is the surface pressure from the normal stress condition, ϕ_a may be any additional pressure applied directly to the surface, ϕ_f is the current value of pressure in the chosen neighboring full cell and η is the previously defined interpolation number.

There are two situations in which the η value used in (3) must be changed. If the calculated length d happens to exceed one and one-half cell widths ($\eta < 2/3$), then η is assigned the value 2/3. This happens, when the line connecting the full and surface cell centers does not intersect the surface within the surface cell; for example, as the surface shown in Fig. 2 is translated upward, the line coming from the full cell on the right intersects the surface more and more to the left, eventually intersecting it outside the surface cell.

When the intersection point lies within the full cell ($\eta > 2$) the pressure iteration will diverge unless a modification is introduced. The pressure in all full cells is allowed to relax during the iteration according to

$$\phi_f^{h+1} = (1 - \omega_0)\, \phi_f{}^h + \omega_0 \tilde{\phi}^h, \tag{4}$$

where ω_0 is a constant relaxation parameter, h refers to the iteration level, and

$$\tilde{\phi}^h = \tfrac{1}{4}(\phi_r{}^h + \phi_t{}^h + \phi_l^{h+1} + \phi_b^{h+1}) + S. \tag{5}$$

The subscripts refer to the neighboring cells at the right, top, left and bottom; S is the usual velocity source term [1]. To maintain stability, the full interpolation cell pressure must be under-relaxed by an amount depending on the value of η. A variable relaxation parameter can be derived for the full interpolation cells that acts as an under-relaxer when $\eta > (5 - 4/\omega_0)$. This relaxation parameter

$$\omega_f = \frac{4\omega_0}{4 - \omega_0(1 - \eta)} \tag{6}$$

is used only with the full interpolation cell. The other full cells use the constant relaxation parameter ω_0, which corresponds to $\eta = 1.0$ in (6). We have found 1.7 or 1.8 to be generally the most effective value for ω_0.

The origin of the η-dependent relaxation factor arose from the observation that divergence was occurring when η exceeded 2, because a change in a full cell pressure could produce a larger change in a neighboring surface cell pressure as calculated by Eq. (3). This then caused the full cell pressure to change by a larger amount, and in the opposite direction, during the next iteration. Repetition of this process in successive iterations resulted in oscillating and diverging pressures. This kind of divergence is avoided, however, if the surface cell pressure used in Eq. (5) is evaluated at the new iteration level $h + 1$. In other words, ϕ_f^{h+1} depends on a surface pressure that must be expressed as a function of ϕ_f^{h+1} itself. Instead of actually doing this, however, the same result can be obtained by using the suggested relaxation parameter together with Eqs. (3)–(5).

Use of the new surface pressure interpolation technique produces a smooth surface and results that closely approximate experimental and analytical data. A comparison of experimental [5] and calculational results, both with and without the interpolation technique, for the surge front of a collapsing fluid column is shown in Figs. 3 and 4. There is excellent agreement between the experimentally measured surge front position as a function of time and a calculation using the interpolation technique. A slower front velocity is calculated with the less accurate, original MAC technique. This is due primarily to the irregular velocities at the surface resulting from incorrect pressures in surface cells. These velocities have created "humps" on what should otherwise be a relatively smooth surface and as a result the front moves too slowly.

In Fig. 5 the cross section of a column of fluid undergoing a steady rotation about an axis at its left side is shown both with and without the new surface treatment. The plots show the calculation, which started with the correct equilibrium solution of a paraboloid of revolution, after 15 cycles. As can be seen in Fig. 5b, equilibrium could not be maintained with the surface treatment used in the original

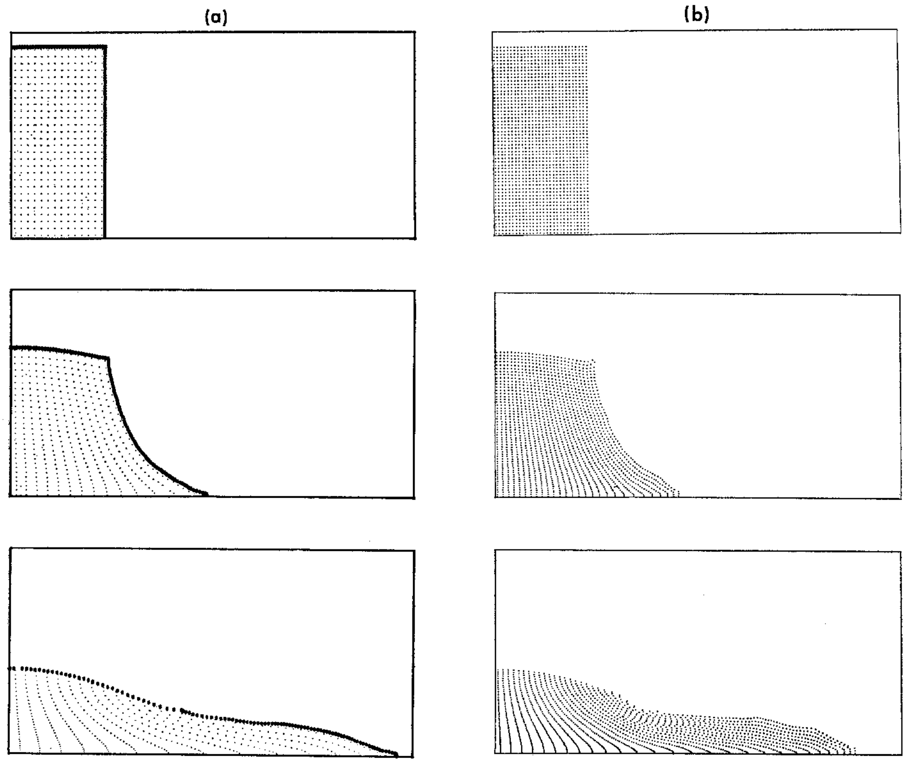

FIG. 3. Comparison of a collapsing fluid column calculated with the surface pressure interpolation scheme (a) and with surface cell pressure equal to zero (b) at times 0., 2., and 4.

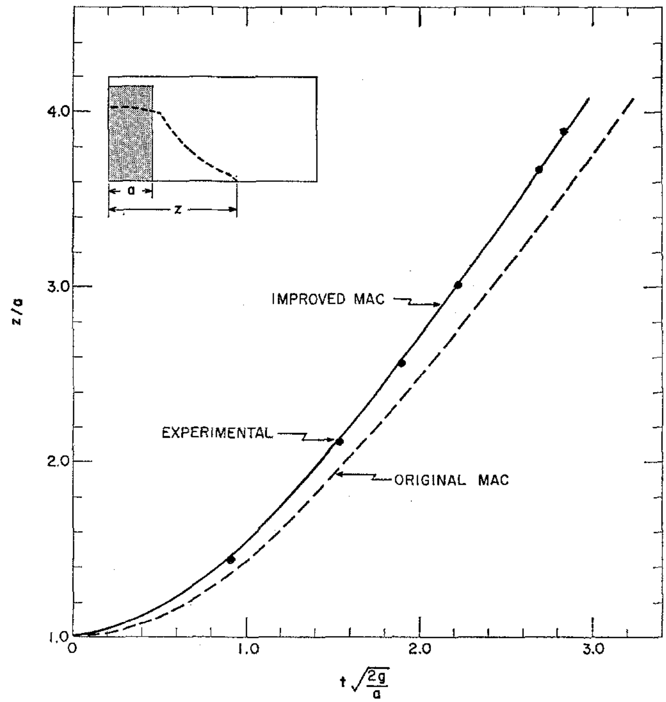

FIG. 4. Comparison of experimental and computer-generated data for the surge front velocity of a collapsing fluid column. The experimental points have been shifted 0.28 units to the left, which is consistent with the uncertainty of the time at which motion began in the experiments.

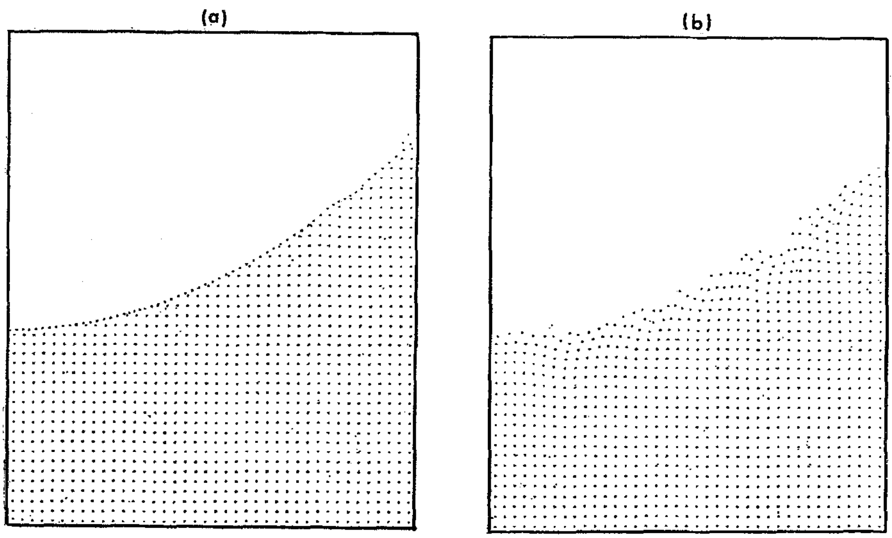

FIG. 5. Cross sections of a fluid column rotating about an axis at its left side with (a) and without (b) the surface pressure interpolation scheme.

MAC method. In Fig. 5a, the relative smoothness of the surface demonstrates the effectiveness of the new method. A slight irregularity, however, is seen in the upper portion of the surface, which results from interpolating the pressure from only one of the two neighboring full cells. The computed surface cell pressure is not precisely correct in relation to the other full cell; consequently, a slightly spurious velocity is induced at the surface. This is most likely to occur when the surface is much closer to one of the full cells than the other.

The splashing drop, as shown in cross section in Fig. 6, points out the capability of the new surface interpolation technique to function when surfaces collide. The Reynolds number of this problem, referring to the radius and initial velocity of the drop, is 75. It is evident from the initial plot that when the drop collides with the pool of fluid, surface particles are going to be "trapped" in the interior of the fluid. These particles are deleted when they end up in full cells, since they serve no useful purpose in such cases. The definition of the surface is retained by adding particles in the gap left by the deletion. These are placed on a straight line connecting the surface particles on each side of the gap. Indeed, any time two successive

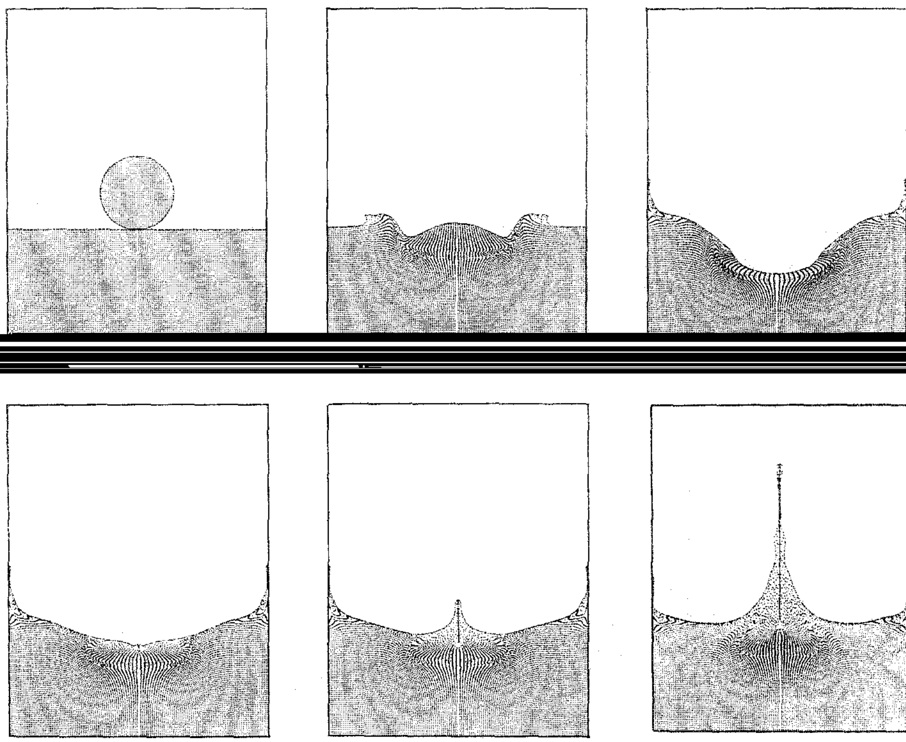

FIG. 6. Cross sections of a splashing drop in a deep pool.

surface marker particles become too far apart, additional particles may be added to adequately maintain definition of the surface. In both the deletion and addition processes, the successive numbering of these particles is required.

Another advantage of the surface pressure interpolation scheme in calculating this kind of problem is evident when compared with similar runs using the original MAC surface treatment. In these earlier calculations, the surface of the collapsing crater becomes irregular resulting in the appearance of holes in the fluid interior [6]. While not entirely detrimental to the calculation, this feature was undesirable and has now been eliminated with the new interpolation scheme. This scheme also prevents the breaking away of spurious particles from the fluid as the crater closes and fluid jets upward in the center, as happened in the original MAC calculations.

The Tangential Stress Condition

Another problem requiring accurate free surface stress conditions is the formation of a viscous bore. The improved accuracy that can be obtained through use of the normal stress condition has been demonstrated for this problem at low Reynolds number flows, even though the surface pressure was then specified at cell center [2]. This initial investigation revealed that without inclusion of the stress conditions the calculated speed of the bore front was greater than the predicted theoretical value, and the height of the fluid behind the bore at the left wall was less, although an overshoot was observed at the front of the bore. The excessive speed of the bore was explained as resulting from the incorrect use of $\phi = 0$ in surface cells at the front of the bore. The pressure should have been positive there because of a viscous contribution. This caused the bore to move forward too rapidly and the fluid height behind the bore to be too low. Inclusion of the normal stress condition did improve the accuracy of the calculation [2]; the bore speed, however, was somewhat less than the theoretical value, and an overshoot in fluid height at the bore front was still observed. These anomalies were then explained as possibly resulting from the use of an incomplete tangential stress condition.

A more correct tangential stress condition is given by Eq. (2). To apply this condition it is again necessary to know the position and shape of the surface. In principle, these can be calculated from the location of the surface marker particles, but because of the other approximations in the MAC method it is sufficient to crudely sense surface slope according to the arrangement of neighboring empty cells, as was done in the previous section. Thus, for a two-dimensional surface, if the surface is nearly horizontal or vertical, the tangential stress condition is

$$\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} = 0; \tag{7}$$

if, however, the surface slope is at 45° to the horizontal, which is approximately the case when there are two adjacent empty cells contiguous to the surface cell, the condition is then

$$\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} = 0. \tag{8}$$

Originally the tangential stress condition was approximated by choosing those velocities needed in cells outside the free surface equal to the corresponding velocities inside the surface, which approximate the condition $\partial u_m / \partial n = 0$. This approximation is not correct at low Reynolds numbers and permits a flux of tangential momentum into the surface at the bore front. It was suggested that such a flux could account for slowing the bore down and contribute to the overshoot in elevation.

We have now included both the normal and tangential stress conditions. In cells with two sides open to empty cells, the original MAC method specified that both $\partial u/\partial x$ and $\partial v/\partial y$ should be individually zero. This then satisfied the tangential stress condition for a 45° surface (8). The only addition needed is a prescription for condition (7). As an example, suppose there are two adjacent surface cells (i, j) and $(i + 1, j)$ that have above them two adjacent empty cells $(i, j + 1)$ and $(i + 1, j + 1)$ (see Fig. 7). The surface would then be horizontal and a prescription for the tangential velocity outside the surface $u^{j+1}_{i+1/2}$ is needed. According to Eq. (7) this velocity is related to those within the fluid by

$$u^{j+1}_{i+1/2} = u^{j}_{i+1/2} - \frac{\delta y}{\delta x}\left(v^{j+1/2}_{i+1} - v^{j+1/2}_{i}\right), \tag{9}$$

where the velocities $v_i^{j+1/2}$ and $v_{i+1}^{j+1/2}$ are determined by requiring the incompres-

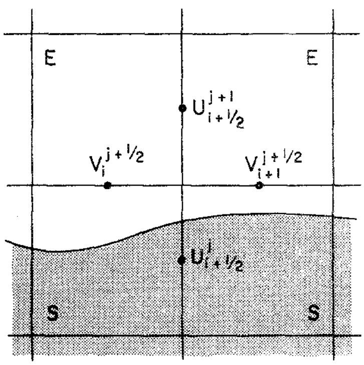

FIG. 7. Tangential velocity selection at a horizontal surface.

sibility condition to be satisfied in surface cells, as was done in the original MAC method. A similar expression can be constructed for a vertical surface.

Actually, this tangential stress condition, and the normal condition involving the viscous term should only be used for sufficiently low Reynolds number flows. We shall return to what constitutes a sufficiently low Reynolds number shortly.

The low Reynolds number ($R = 4.33$), viscous bore calculation has been repeated with the full stress conditions. An exact comparison with the earlier work is not made because the code used for these calculations does not have a fluid input boundary condition at the right wall, which allowed a continuing input of fluid to sustain the bore formation in the earlier calculations. To partially overcome this, a mesh twice as long as the original was used. The remainder of the initial conditions were the same. The plots shown in Fig. 8 present only the left half of the calculational mesh. The comparison of results is made at a time to assure adequate fluid for the proper bore formation. As was postulated [2], the inclusion of the tangential stress conditions did improve the bore speed, which is

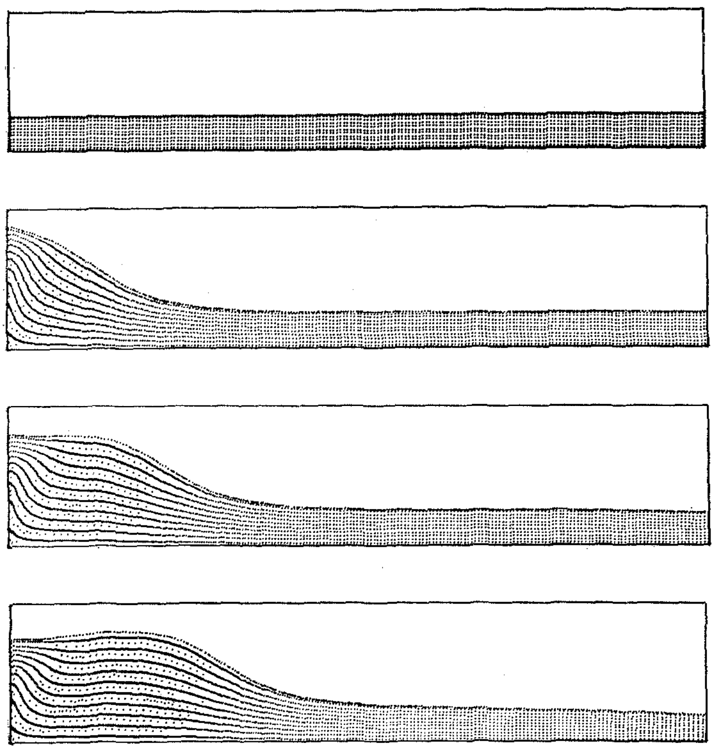

FIG. 8. Viscous bore ($R = 4.33$) calculated with full stress conditions. Configurations shown are at times 0., 3., 4.6, and 6.

now nearly equal to the theoretical value of 0.577. It is calculated to be 0.575 to a time of approximately 6. At later times the incoming fluid height is slightly less than it should be and the bore speed drops off.

With the full stress conditions, the bore height at the left wall is still not equal to the theoretical value of 1.50. The fluid depth at the left wall was only raised from 1.40 to 1.41 by including the tangential stress conditions; however, with the addition of the surface pressure interpolation technique, the depth was raised to 1.47. This level is approached asymptotically. The avarage height of the bore front and the fluid at the left wall is approximately 1.50, which is consistent with the conservation of mass, as it must be. It had been assumed that with the correct pressure defined in surface cells the overshoot in height at the bore front would disappear. This did not occur which suggests that such an overshoot is physically correct. However, it may be that a still more refined treatment of the tangential stress condition would eventually eliminate this overshoot.

Now that a complete set of free surface stress conditions have been incorporated into the MAC method, it must be pointed out that they cannot be used indiscriminately for all calculations. Some hint of this can be gleaned from the observation that the tangential stress condition (2) is unnecessary for inviscid problems ($\nu = 0$), but the numerical approximation (9) is independent of ν. This situation can be better understood by first considering a related problem.

At a rigid wall the tangential stress condition requires that the fluid not slip along the wall. In an actual fluid this implies the development of a boundary layer, in which the fluid is accelerated from the wall velocity to a free stream value some distance from the wall. The thickness of the boundary layer may be large or small with respect to an Eulerian cell dimension, depending on the problem under consideration. An estimate of when a thick or thin boundary layer should be observed can be obtained from the following argument. Let U and L be a typical velocity and dimension in the problem of interest. According to simple boundary layer theory, the boundary layer thickness, developed along a wall of length L, is proportional to $\sqrt{\nu L/U}$. If it is assumed that a typical linear dimension L is resolved by N finite difference intervals, i.e., $L = N\delta x$, then the boundary layer will be small with respect to a cell dimension, provided $R \gg N^2$, where $R = UL/\nu$ is the flow Reynolds number. Thus, the boundary layer is "thin" when the flow Reynolds number is much larger than the square of the number of cells resolving a typical length L.

Figure 9 schematically shows a velocity profile with a boundary layer much thinner than a cell width $R \gg N^2$. In this case choosing the value of u_{out} to be equal to u_{in} (leading to vertical dashed line in Fig. 9), rather than the negative of u_{in} (leading to diagonal dashed line in Fig. 9), offers a better approximation to the velocity profile near the wall. The no-slip condition in this case ($u_{\text{out}} = -u_{\text{in}}$) forces an artificially large drag on the fluid, while the free-slip condition ($u_{\text{out}} = u_{\text{in}}$)

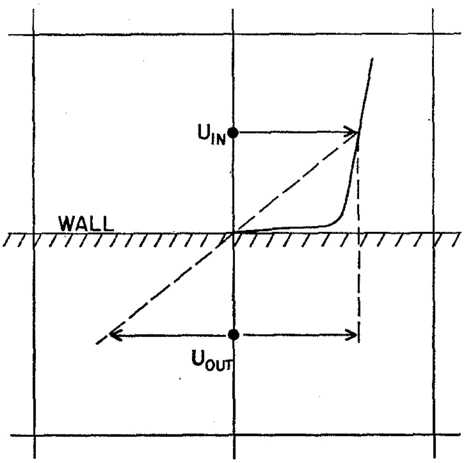

FIG. 9. Velocity profile for a thin boundary layer.

represents no boundary drag, clearly a much better approximation. Actually one might argue that the no-slip condition could be used all the time, since a thin boundary layer occurs only when viscous effects are small, in which case it should not matter what is done with u_{out}. Unfortunately, it is often necessary for computational stability to use a viscosity that is larger than that for a real fluid. In such cases it is necessary to use the free slip prescription to prevent an unrealistically large transfer of tangential momentum from the wall.

If the boundary layer is thick with respect to a cell width $R < N^2$, then a significant tangential momentum transfer should occur at the wall and the no-slip condition is the correct boundary condition.

At a free surface the situation is much the same. When the fluid is treated as nearly inviscid it is incorrect to use the complete free surface stress conditions. Instead, the inviscid condition $\phi = 0$ should be applied at the surface, and all velocities needed outside a surface should be obtained by extrapolating interior values outward.

NUMERICAL STABILITY CONSIDERATIONS

There are unique numerical instabilities associated with each of the iteration sequences in MAC calculations, i.e., with the pressure iteration at a given time step and with the successive steps of time advancement. Both kinds of iteration stability criteria are affected by use of the surface pressure interpolation technique and by the stress conditions.

As previously pointed out, a variable relaxation parameter is necessary to prevent instability within the pressure iteration scheme. Otherwise, a flip-flop growth of pressures will occur due to an excessive feedback between surface and full cells.

Another potential source of numerical instability is the viscous diffusion terms in the finite-difference momentum equations. In the original MAC method the condition necessary to insure stability through successive time steps was

$$\nu \delta t < \frac{1}{2} \left(\frac{\delta x^2 \, \delta y^2}{\delta x^2 + \delta y^2} \right). \tag{10}$$

This condition, the derivation of which is discussed in Ref. 1, must be modified to include a dependence on the interpolation number η when the normal and tangential stress conditions are employed.

The dependence of this numerical stability criterion on the inclusion of the normal stress condition can be demonstrated in the following way. Consider the velocity profile in the neighborhood of a pair of surface cells as shown in Fig. 10. The velocities at the top of each surface cell have been chosen such that there is a zero net mass flux into each cell, in accord with the usual MAC prescription. As a result, all velocities in the figure have equal magnitudes. The tangential stress condition requires the $u_{\text{out}} = -u_{\text{in}}$. The change in u_{in} during the next time step is easy to compute, and is found to change sign. The requirement that the new

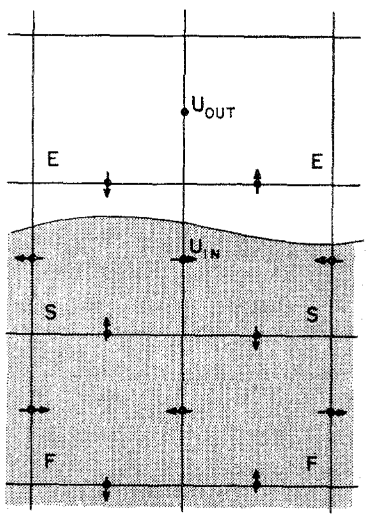

FIG. 10. Velocity profile for the numerical stability criterion model.

magnitude of u_{in} be no larger than it was before the change leads to the requirement (with $\delta x = \delta y$)

$$\frac{\nu \delta t}{\delta x^2} < \frac{1}{4\eta + 4}. \tag{11}$$

If this condition is violated the u-velocity will oscillate in sign and grow in magnitude on successive time cycles, leading to a familiar kind of numerical instability. This simple model of instability at a free surface is likely to be the worst case, because it involves the shortest wave length disturbance resolvable in the mesh and this is generally the most likely to be affected by viscous effects. Clearly, the value of η can not be too large if stability is to be maintained. In practice the limitation $\eta \lesssim 2$ has had little adverse effect on the calculational results to which it has been applied.

If the Reynolds number of the flow is large enough, the stress conditions should be applied as for an inviscid fluid, in which case the stability condition (11) can be relaxed to

$$\frac{\nu \delta t}{\delta x^2} < \frac{1}{3}. \tag{12}$$

Actually, the velocity distribution shown in Fig. 10 is unstable away from the surface unless $\nu\delta t/\delta x^2 < \frac{1}{4}$. Therefore, the dominant influence of the new stress conditions arrives from the magnification of the normal stress condition by the interpolation factor η, and this only in the neighborhood of the surface.

Acknowledgments

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