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Transport of Turbulence in Numerical Fluid Dynamics

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ABSTRACT

Recently proposed turbulence transport equations have been incorporated into the Marker-and-Cell method for the numerical calculation of transient flows of viscous incompressible fluids. The results account automatically for the creation, convection, diffusion, and decay of turbulence and for the effects of the turbulence on the mean flow.

INTRODUCTION

The Marker-and-Cell (MAC) method [1]–[3] has been used to solve numerically a wide variety of problems concerning the transient dynamics of viscous incompressible fluids in several space dimensions. Examples include the splash of a liquid drop [4], [5], surge wave formation from the release of water behind a sluice gate [6], the flow of density currents [7], formation of a von Kármán vortex street [8], and Rayleigh–Taylor instability of a two-fluid system [9].

Some of the examples demonstrate the early stages of transition to turbulence, but it has become clear that fully developed turbulence cannot be calculated in the near future because of resolution limitations on all presently available computers. The situation resembles that of gas dynamics itself in which the calculation of individual molecular trajectories would be a hopeless task in any but the most limited circumstances.

The familiar alternative for fluid-flow studies is to introduce some mean properties of the molecular dynamics; these are such field variables as mean velocity, pressure, temperature, and viscous stress. For turbulence, a recent proposal [10], [11] is closely analogous. The effects of turbulence are represented by a set of field variables expressing the required mean properties of the detailed fluctuations, and for these turbulence field variables there are corresponding transport equations describing the Eulerian variations in terms of appropriate creation, convection, diffusion, and decay terms.

The turbulence transport equations are of considerable complexity, so that analytical solutions are now possible only for a small number of specialized circumstances. Accordingly, their greatest utility comes from incorporation into a numerical method (such as MAC) for the solution of fluid dynamics problems, and utilizing the available high-speed computers. The purpose of this paper is to describe such a combination of techniques by which turbulence can be represented with considerable accuracy for both transient and steady-state problems. We also show that turbulence introduces diffusive effects that stabilize the numerical calculations at high Reynolds numbers, thereby extending considerably the usefulness of the MAC technique without the necessity of introducing implicit or explicit artificial diffusive stabilizers. The present paper is formulated for problems with no appreciable dynamics in regions of very weak turbulence, for which additional complications arise.

The Equations

The complete set of differential equations contains the incompressibility condition

$$\frac{\partial u_k}{\partial x_k} = 0, \tag{1}$$

the momentum equation

$$\frac{\partial u_j}{\partial t} + u_k \frac{\partial u_j}{\partial x_k} = g_j - \frac{\partial}{\partial x_j}\left(\varphi + \frac{2}{3} q\right) + \frac{\partial}{\partial x_k}[(\nu + \sigma)\, e_{jk}], \tag{2}$$

the turbulence energy equation

$$\frac{\partial q}{\partial t} + u_k \frac{\partial q}{\partial x_k} = \sigma e_{jk} \frac{\partial u_j}{\partial x_k} + \frac{\theta}{\gamma} \frac{\partial}{\partial x_k}\left(\sigma \frac{\partial \varphi}{\partial x_k}\right) + \frac{\partial}{\partial x_k}\left[(\nu + \alpha\sigma) \frac{\partial q}{\partial x_k}\right] - 2\nu\mathscr{D}, \tag{3}$$

the decay-term equation

$$\frac{\partial \mathscr{D}}{\partial t} + u_k \frac{\partial \mathscr{D}}{\partial x_k} = \frac{a\Delta\sigma}{s^2} e_{jk} \frac{\partial u_j}{\partial x_k} - \frac{2\nu\Delta'\mathscr{D}}{s^2} + \frac{a_2\Delta}{s^2} \frac{\partial}{\partial x_k}\left(\sigma \frac{\partial q}{\partial x_k}\right) + \frac{\partial}{\partial x_k}\left[(\nu + a_3\sigma) \frac{\partial \mathscr{D}}{\partial x_k} + \frac{a_4\Delta\sigma}{s^2} \frac{\partial \varphi}{\partial x_k}\right], \tag{4}$$

together with the relationships

$$q = \frac{1}{2\gamma}\left(\frac{\sigma}{s}\right)^2, \tag{5}$$

$$\mathscr{D} = \frac{\Delta q}{s^2}, \tag{6}$$

$$\Delta = \beta(1 + \delta\sigma/\nu), \tag{7}$$

$$\Delta' = \beta'(1 + \delta'\sigma/\nu). \tag{8}$$

Here, u_k is the component of mean velocity in the direction of x_k, g_j is the gravitational acceleration, φ is the ratio of mean pressure to (constant) density, q is the turbulence kinetic energy per unit mass, ν is the (constant) molecular kinematic viscosity coefficient, σ is the (variable) turbulence kinematic viscosity coefficient, e_{jk} is the rate-of-strain tensor ($e_{jk} \equiv \partial u_j/\partial x_k + \partial u_k/\partial x_j$), $\mathscr{D}$ is the turbulence energy decay function, $(\Delta)^{1/2}$ is proportional to the ratio between turbulence integral scale and turbulence microscale, and s is proportional to the turbulence integral scale (but equal to the microscale in the limit of weak turbulence). In addition, there are several dimensionless, universal constants, of which α, γ, θ, and a_3 are near unity, $\beta = 5$ and $\beta' \approx 10$, a is slightly less than 2.0, a_2 and a_4 are small or zero, while δ and δ' are of the order of 0.2. The probable values and significances of the various constants are discussed in several other publications [10], [12].

These, then, are the equations to be solved. They are tensor invariant, Galilean invariant, rotationally invariant, and universal in the sense that the coefficients are not problem-dependent. Thus, it is possible to incorporate them into a numerical solution technique with the expectation of broad applicability.

Their principal limitation is implied by the scalar turbulence viscosity function, which means decreasing accuracy as non-isotropy increases. (Tests in problems with strong non-isotropy, however, show that this is not as serious a limitation as might be expected [10], [12].)

The initial conditions for these equations describe the state of the mean flow, together with the initial "noise" level. If $\sigma \equiv 0$ at $t = 0$, then turbulence can never occur. For problems in which only the steady state is of interest, the initial value of σ is otherwise of no significance. In transient problems both σ and s (or functions thereof) must be available to completely specify the initial state; unfortunately, many experimentalists have only measured q in their initial flow, so that complete specification is seldom available for such comparison calculations, and the initial scale, for example, must be guessed on the basis of plausibility arguments.

The boundary conditions at a rigid, no-slip wall are such that σ and s both vanish, and also $q = 0$, $\mathscr{D} = 0$. [The vanishing of $\mathscr{D}$ follows from Eq. (4), in that the decay term in that equation would approach $(-\infty)$ at a wall if $\mathscr{D}$ did not there vanish, and the decay of $\mathscr{D}$ to zero would take place immediately.] In numerical calculations, free-slip walls are also of interest for two purposes. They represent truly no-slip walls for circumstances in which the expected boundary layer is much narrower than the finite-difference zones. They also are convenient as lines of symmetry, in which only half of a symmetric or antisymmetric flow region need be calculated. Free-slip-wall boundary conditions are determined by specifying that the reflected flow region be the same or the reflection of that on the calculated side of the wall.

One aspect of the initial conditions for these finite-difference calculations of turbulence reflects crucially upon the basic interpretations of the turbulence transport theory itself. This is the question: Which part of the detailed flow should be called the turbulence fluctuations and which part should be called the mean flow? In other words: Would we get the same result from two calculations in which

(a) the large eddies are resolved as part of the mean flow, or

(b) the large eddies are not resolved but instead absorbed into the values of σ and s?

Two considerations reflect upon the answers to these questions. First, the specification of σ and s for a particular field of turbulence implies a local spectrum (like a slightly-perturbed Maxwell–Boltzmann molecular-velocity distribution) which departs only to lowest order from a local equilibrium spectrum. Thus the resolved large-scale structure must represent that part of the spectrum that departs *strongly* from this assumed near equilibrium, forming, at least in principle, a criterion for separating the detailed flow into the turbulent and mean parts.

The second consideration concerns the transport of *total* kinetic energy, both mean and turbulent. Let q_{T} be that total. Then the differential equations can be combined to show that

$$\frac{\partial q_{\mathrm{T}}}{\partial t} + u_k \frac{\partial q_{\mathrm{T}}}{\partial x_k} = g_j u_j - \nu \overline{\left[\frac{\partial(u_j + u_j')}{\partial x_k}\right]^2} + \frac{\partial}{\partial x_k}\left[\frac{\theta\sigma}{\gamma}\frac{\partial\varphi}{\partial x_k} - u_k(\varphi + \frac{2}{3}q) + \sigma\frac{\partial u_j u_k}{\partial x_j} + (\nu + \sigma)\frac{\partial q_{\mathrm{T}}}{\partial x_k}\right],$$

where u_j' is the fluctuating part of the flow and the bar implies ensemble average. Thus we conclude that the transport of *total* kinetic energy is "nearly" independent of the division into mean and turbulence parts.

Fluctuating laminar flows (from laminar instability) require additional interpretive considerations. These can be represented by the turbulence field variable theory only with the inclusion of several additional features [13]. In the present formulation, they are to be considered part of the mean flow.

The Basic MAC Method

The basic MAC technique has been described in detail elsewhere [1], [3], so that only a brief review will be given here.

The computational region in MAC is based on a rectangular mesh of fixed Eulerian cells through which the fluid moves, along with a set of marker particles to denote the fluid configuration. As described here, we are concerned with two-dimensional Cartesian coordinates and a single fluid that fills the mesh, although the method has been successfully applied to problems involving several distinct fluids [3], [7], [9], free-surface flows [2], [4], and has been extended to cylindrical geometry [5], [6]. To achieve this versatility, the method is based upon pressure and velocity as the primary variables, rather than the vorticity and stream function. This is of advantage particularly in the application of the free surface boundary condition of vanishing or prescribed normal stress. It is also an aid in visualizing the physical significance of the results and of any extensions to the basic technique.

The x and y coordinate axes of the MAC mesh are horizontal and vertical, respectively, with the origin located at the lower left corner of the computing region. The corresponding velocity components are u and v, while φ is the ratio of pressure to (constant) density, although we simply refer to φ as "pressure."

In our finite-difference approximation, the cells are numbered by the indices i and j, which count cell center positions in the horizontal and vertical directions respectively. Cell boundary positions are thus labeled with half-integer values of the indices. The rectangular cells are of dimensions δx by δy. The placement of the local field variables is shown in Fig. 1.

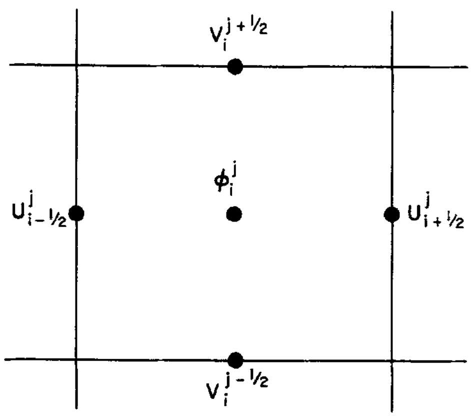

FIG. 1. Placement of field variables about a MAC cell. Pressure is defined at the cell center, and velocities are defined on the cell boundaries.

The calculation proceeds through a sequence of time cycles, each advancing the entire fluid configuration through a small but finite increment of time δt.

The derivation of the finite difference equations is based upon the following sequence of events, which advance the fluid configuration from one time step to the next.

The complete velocity field is known at the beginning of the cycle, either from the initial conditions or as a result of the previous cycle of calculation. This velocity field is conservative in that the finite-difference analogy of velocity divergence vanishes for every cell.

First, the pressure for each cell is obtained by solving a finite-difference Poisson's equation which satisfies the incompressibility condition, and whose source term is a function of the velocities.

Second, the full finite-difference Navier–Stokes equations are used to find the new velocities throughout the mesh.

Third, the marker particles are moved with a weighted average of the four nearest cell velocities. Particles may be created at an input boundary or destroyed at an output boundary as required. For confined-flow problems, the marker particles do not enter directly into the calculation but are used merely to define the fluid configuration. For free-surface flows they show which cells are on the surface and therefore need special treatment.

Finally, boundary condition values are adjusted in such a way that the next cycle can begin. The time counter is advanced, and results are printed or plotted as desired.

Since the results of each cycle act as initial conditions for the next one, the calculation may be continued for as many cycles as necessary to develop the solution. In particular, the development of large-amplitude distortions or free surfaces folding back on themselves have no adverse effects on the accuracy or calculability of the problem.

Turbulent Transport in MAC

The specialization of turbulence transport effects in two space dimensions to MAC is primarily manifested in the addition of new terms in the MAC momentum equations, plus equations for $\mathscr{E}$ ($\equiv \sigma^2/s^2$) and DISS [$\equiv (2\gamma/\beta)\,\mathscr{D}$]. The basic differential equations for this form of MAC are specialized from Eqs. (1)–(8):

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \tag{9}$$

$$\frac{\partial u}{\partial t} + \frac{\partial u^2}{\partial x} + \frac{\partial uv}{\partial y} = g_x - \frac{\partial(\varphi + \frac{2}{3}q)}{\partial x} + \frac{\partial}{\partial x_k}\left[(\nu + \sigma)\, e_{xk}\right], \tag{10}$$

$$\frac{\partial v}{\partial t} + \frac{\partial v^2}{\partial y} + \frac{\partial uv}{\partial x} = g_y - \frac{\partial(\varphi + \frac{2}{3}q)}{\partial y} + \frac{\partial}{\partial x_k}\left[(\nu + \sigma)\, e_{yk}\right], \tag{11}$$

$$\frac{\partial \mathscr{E}}{\partial t} + \frac{\partial u\mathscr{E}}{\partial x} + \frac{\partial v\mathscr{E}}{\partial y} = 2\gamma\sigma \left[\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + 2\left(\frac{\partial u}{\partial x}\right)^2 + 2\left(\frac{\partial v}{\partial y}\right)^2\right]$$
$$+ 2\theta \left[\frac{\partial}{\partial x}\left(\sigma \frac{\partial \varphi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\sigma \frac{\partial \varphi}{\partial y}\right)\right] - 2\beta\nu\, DISS$$
$$+ \frac{\partial}{\partial x}\left[(\nu + \alpha\sigma)\frac{\partial \mathscr{E}}{\partial x}\right] + \frac{\partial}{\partial y}\left[(\nu + \alpha\sigma)\frac{\partial \mathscr{E}}{\partial y}\right], \tag{12}$$

$$\frac{\partial\, DISS}{\partial t} + \frac{\partial u\, DISS}{\partial x} + \frac{\partial v\, DISS}{\partial y}$$
$$= \frac{2\gamma a\sigma\Delta}{s^2\beta}\left[2\left(\frac{\partial u}{\partial x}\right)^2 + 2\left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2\right]$$
$$- \frac{2\nu\Delta'\, DISS}{s^2} + \frac{a_2\Delta}{s^2\beta}\left[\frac{\partial}{\partial x}\left(\sigma\frac{\partial \mathscr{E}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\sigma\frac{\partial \mathscr{E}}{\partial y}\right)\right]$$
$$+ \frac{\partial}{\partial x}\left[(\nu + a_3\sigma)\frac{\partial\, DISS}{\partial x}\right] + \frac{\partial}{\partial y}\left[(\nu + a_3\sigma)\frac{\partial\, DISS}{\partial y}\right]$$
$$+ 2\gamma a_4\left[\frac{\partial}{\partial x}\left(\frac{\sigma\Delta}{s^2\beta}\frac{\partial\varphi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\sigma\Delta}{s^2\beta}\frac{\partial\varphi}{\partial y}\right)\right], \tag{13}$$

where Eq. (9) is the incompressibility condition, Eqs. (10) and (11) are the momentum equations, and Eqs. (12) and (13) are the turbulence transport equations. In what follows, we take $\delta' = \delta$. This restriction, together with the simple transport flux forms used here, imply restriction from problems with very weak turbulence, $\sigma/\nu \lesssim 10$, as described in Ref. 13.

It should be mentioned that we have found it useful to base the nonturbulent MAC difference equations on the viscous term $-\nu\nabla \times \nabla \times \mathbf{u}$ rather than $\nu\nabla^2\mathbf{u}$, as had been used in the early MAC technique publications. The result is considerable simplification, rather than increased accuracy. The analogous form to the "double-curl" differencing is also used in the following difference equations with turbulence.

Our finite-difference approximations use a left-side superscript to denote the time cycle, in addition to the right-side i and j space-indexing subscript and superscript. Thus, the horizontal velocity at the time $t = (n + 1)\,\delta t$ would be designated ${}^{n+1}u^j_{i-1/2}$. When the cycle-number index is omitted, it is assumed to be n, the value of the quantity at the beginning of the cycle.

The finite-difference approximations to Eqs. (10) through (13) are written in the following form:

$$
\begin{aligned}
{}^{n+1}u^{j}_{i-1/2} = {}^{n}u^{j}_{i-1/2} + \delta t \Bigg\{ & \frac{(u^{j}_{i-1})^2 - (u_i^{\,j})^2}{\delta x} + \frac{(uv)^{j-1/2}_{i-1/2} + (uv)^{j+1/2}_{i-1/2}}{\delta y} \\
& + g_x + \frac{\Phi^{j}_{i-1} - \Phi_i^{\,j}}{\delta x} \\
& - \frac{2}{\delta x \delta y} [(\nu + \sigma_i^{\,j})(v_i^{j+1/2} - v_i^{j-1/2}) - (\nu + \sigma^{j}_{i-1})(v^{j+1/2}_{i-1} - v^{j-1/2}_{i-1})] \\
& + \frac{1}{\delta y} \Bigg[(\nu + \sigma^{j+1/2}_{i-1/2}) \left(\frac{u^{j+1}_{i-1/2} - u^{j}_{i-1/2}}{\delta y} + \frac{v_i^{j+1/2} - v^{j+1/2}_{i-1}}{\delta x} \right) \\
& - (\nu + \sigma^{j-1/2}_{i-1/2}) \left(\frac{u^{j}_{i-1/2} - u^{j-1}_{i-1/2}}{\delta y} + \frac{v_i^{j-1/2} - v^{j-1/2}_{i-1}}{\delta x} \right) \Bigg] \Bigg\},
\end{aligned}
\tag{14}
$$

$$
\begin{aligned}
{}^{n+1}v_i^{j-1/2} = {}^{n}v_i^{j-1/2} + \delta t \Bigg\{ & \frac{(v_i^{j-1})^2 - (v_i^{\,j})^2}{\delta y} + \frac{(uv)^{j-1/2}_{i-1/2} - (uv)^{j-1/2}_{i+1/2}}{\delta x} \\
& + g_y + \frac{\Phi_i^{j-1} - \Phi_i^{\,j}}{\delta y} \\
& - \frac{2}{\delta x \delta y} [(\nu + \sigma_i^{\,j})(u^{j}_{i+1/2} - u^{j}_{i-1/2}) - (\nu + \sigma_i^{j-1})(u^{j-1}_{i+1/2} - u^{j-1}_{i-1/2})] \\
& + \frac{1}{\delta x} \Bigg[(\nu + \sigma^{j-1/2}_{i+1/2}) \left(\frac{u^{j}_{i+1/2} - u^{j-1}_{i+1/2}}{\delta y} + \frac{v^{j-1/2}_{i+1} - v_i^{j-1/2}}{\delta x} \right) \\
& - (\nu + \sigma^{j-1/2}_{i-1/2}) \left(\frac{u^{j}_{i-1/2} - u^{j-1}_{i-1/2}}{\delta y} + \frac{v_i^{j-1/2} - v^{j-1/2}_{i-1}}{\delta x} \right) \Bigg] \Bigg\},
\end{aligned}
\tag{15}
$$

$$
\begin{aligned}
{}^{n+1}\mathscr{E}_i^{j} = {}^{n}\mathscr{E}_i^{\,j} + \delta t \Bigg\{ & \frac{(u\mathscr{E})^{j}_{i-1/2} - (u\mathscr{E})^{j}_{i+1/2}}{\delta x} + \frac{(v\mathscr{E})_i^{j-1/2} - (v\mathscr{E})_i^{j+1/2}}{\delta y} \\
& + 2\gamma\sigma_i^{\,j} \Bigg[\left(\frac{u_i^{j+1/2} - u_i^{j-1/2}}{\delta y} + \frac{v^{j}_{i+1/2} - v^{j}_{i-1/2}}{\delta x} \right)^2 + 2 \left(\frac{u^{j}_{i+1/2} - u^{j}_{i-1/2}}{\delta x} \right)^2 \\
& + 2 \left(\frac{v_i^{j+1/2} - v_i^{j-1/2}}{\delta y} \right)^2 \Bigg] - 2\beta\nu\, DISS_i^{\,j} \\
& + \frac{2\theta}{\delta x^2} [\sigma^{j}_{i+1/2}(\varphi^{j}_{i+1} - \varphi_i^{\,j}) - \sigma^{j}_{i-1/2}(\varphi_i^{\,j} - \varphi^{j}_{i-1})] \\
& + \frac{2\theta}{\delta y^2} [\sigma_i^{j+1/2}(\varphi_i^{j+1} - \varphi_i^{\,j}) - \sigma_i^{j-1/2}(\varphi_i^{\,j} - \varphi_i^{j-1})] \\
& + \frac{1}{\delta x^2} [(\nu + \alpha\sigma^{j}_{i+1/2})(\mathscr{E}^{j}_{i+1} - \mathscr{E}_i^{j}) - (\nu + \alpha\sigma^{j}_{i-1/2})(\mathscr{E}_i^{j} - \mathscr{E}^{j}_{i-1})] \\
& + \frac{1}{\delta y^2} [(\nu + \alpha\sigma_i^{j+1/2})(\mathscr{E}_i^{j+1} - \mathscr{E}_i^{j}) - (\nu + \alpha\sigma_i^{j-1/2})(\mathscr{E}_i^{j} - \mathscr{E}_i^{j-1})] \Bigg\},
\end{aligned}
\tag{16}
$$

$$
\begin{aligned}
{}^{n+1}DISS_i^j = {}^{n}DISS_i^j + \delta t \Bigg\{ & \frac{(u\,DISS)_{i-1/2}^j - (u\,DISS)_{i+1/2}^j}{\delta x} \\
& + \frac{(v\,DISS)_i^{j-1/2} - (v\,DISS)_i^{j+1/2}}{\delta y} \\
& + 2\gamma a\left(\frac{\Delta\sigma}{s^2\beta}\right)_i^j \left[2\left(\frac{u_{i+1/2}^j - u_{i-1/2}^j}{\delta x}\right)^2 + 2\left(\frac{v_i^{j+1/2} - v_i^{j-1/2}}{\delta y}\right)^2\right. \\
& \left. + \left(\frac{u_i^{j+1/2} - u_i^{j-1/2}}{\delta y} + \frac{v_{i+1/2}^j - v_{i-1/2}^j}{\delta x}\right)^2\right] - \frac{2\nu\beta'}{\beta^2}\left(\frac{\Delta^2\sigma^2}{s^6}\right)_i^j \\
& + \left(\frac{\Delta a_2}{s^2\beta}\right)_i^j \left[\frac{\sigma_{i+1/2}^j(\mathscr{E}_{i+1}^j - \mathscr{E}_i^j) - \sigma_{i-1/2}^j(\mathscr{E}_i^j - \mathscr{E}_{i-1}^j)}{\delta x^2}\right. \\
& \left. + \frac{\sigma_i^{j+1/2}(\mathscr{E}_i^{j+1} - \mathscr{E}_i^j) - \sigma_i^{j-1/2}(\mathscr{E}_i^j - \mathscr{E}_i^{j-1})}{\delta y^2}\right] \\
& + \frac{1}{\delta x^2}\Bigg\{\frac{2\gamma a_4}{\beta}\left[\left(\frac{\Delta\sigma}{s^2}\right)_{i+1/2}^j(\varphi_{i+1}^j - \varphi_i^j) - \left(\frac{\Delta\sigma}{s^2}\right)_{i-1/2}^j(\varphi_i^j - \varphi_{i-1}^j)\right] \\
& + (\nu + a_3\sigma_{i+1/2}^j)(DISS_{i+1}^j - DISS_i^j) \\
& - (\nu + a_3\sigma_{i-1/2}^j)(DISS_i^j - DISS_{i-1}^j)\Bigg\} \\
& + \frac{1}{\delta y^2}\Bigg\{\frac{2\gamma a_4}{\beta}\left[\left(\frac{\Delta\sigma}{s^2}\right)_i^{j+1/2}(\varphi_i^{j+1} - \varphi_i^j) - \left(\frac{\Delta\sigma}{s^2}\right)_i^{j-1/2}(\varphi_i^j - \varphi_i^{j-1})\right] \\
& + (\nu + a_3\sigma_i^{j+1/2})(DISS_i^{j+1} - DISS_i^j) \\
& - (\nu + a_3\sigma_i^{j-1/2})(DISS_i^j - DISS_i^{j-1})\Bigg\}\Bigg\}. \qquad (17)
\end{aligned}
$$

We have introduced Φ as the "*total*" pressure, $\Phi \equiv \varphi + \frac{2}{3}q$.

The variables, Φ, σ, and s are defined at cell centers. Note that in the above equations, values of certain variables are not centered at the points where they are normally defined. In such cases an average of adjacent values is implied. As examples,

$$(u_i^j)^2 \equiv \left(\frac{u_{i-1/2}^j + u_{i+1/2}^j}{2}\right)^2,$$

$$\sigma_{i+1/2}^{j-1/2} \equiv \frac{1}{4}(\sigma_i^j + \sigma_{i+1}^j + \sigma_i^{j-1} + \sigma_{i+1}^{j-1}),$$

$$(uv)_{i-1/2}^{j-1/2} \equiv \left(\frac{u_{i-1/2}^j + u_{i-1/2}^{j-1}}{2}\right)\left(\frac{v_i^{j-1/2} + v_{i-1}^{j-1/2}}{2}\right).$$

Now, to satisfy the incompressibility condition, we want

$$^{n+1}D_i^j = 0,$$

which is the finite-difference analog of Eq. (9), in which

$$D_i^j \equiv \frac{u_{i+1/2}^j - u_{i-1/2}^j}{\delta x} + \frac{v_j^{j+1/2} - v_i^{j-1/2}}{\delta y}. \tag{18}$$

If we use Q_i^j as an abbreviation for

$$Q_i^j \equiv \left[\frac{(u_{i+1}^j)^2 + (u_{i-1}^j)^2 - 2(u_i^j)^2}{\delta x^2}\right] + \left[\frac{(v_i^{j+1})^2 + (v_i^{j-1})^2 - 2(v_i^j)^2}{\delta y^2}\right]$$
$$+ 2\left[\frac{(uv)_{i+1/2}^{j+1/2} + (uv)_{i-1/2}^{j-1/2} - (uv)_{i+1/2}^{j-1/2} - (uv)_{i-1/2}^{j+1/2}}{\delta x\, \delta y}\right], \tag{19}$$

and

$$\Omega^2\Phi_i^j \equiv \frac{\Phi_{i+1}^j + \Phi_{i-1}^j - 2\Phi_i^j}{\delta x^2} + \frac{\Phi_i^{j+1} + \Phi_i^{j-1} - 2\Phi_i^j}{\delta y^2},$$

and also define

$$\begin{aligned}
W_i^j = \frac{2}{\delta x^2 \delta y} & [v_{i+1}^{j+1/2}(\sigma_{i+1/2}^{j+1/2} - \sigma_{i+1}^j) + v_{i+1}^{j-1/2}(\sigma_{i+1}^j - \sigma_{i+1/2}^{j-1/2}) \\
& + v_i^{j+1/2}(2\sigma_i^j - \sigma_{i+1/2}^{j+1/2} - \sigma_{i-1/2}^{j+1/2}) + v_i^{j-1/2}(\sigma_{i+1/2}^{j-1/2} + \sigma_{i-1/2}^{j-1/2} - 2\sigma_i^j) \\
& + v_{i-1}^{j+1/2}(\sigma_{i-1/2}^{j+1/2} - \sigma_{i-1}^j) + v_{i-1}^{j-1/2}(\sigma_{i-1}^j - \sigma_{i-1/2}^{j-1/2})] \\
& + \frac{2}{\delta x \delta y^2}[u_{i+1/2}^{j+1}(\sigma_{i+1/2}^{j+1/2} - \sigma_i^{j+1}) + u_{i-1/2}^{j+1}(\sigma_i^{j+1} - \sigma_{i-1/2}^{j+1/2}) \\
& + u_{i+1/2}^j(2\sigma_i^j - \sigma_{i+1/2}^{j+1/2} - \sigma_{i+1/2}^{j-1/2}) + u_{i-1/2}^j(\sigma_{i-1/2}^{j-1/2} + \sigma_{i-1/2}^{j+1/2} - 2\sigma_i^j) \\
& + u_{i+1/2}^{j-1}(\sigma_{i+1/2}^{j-1/2} - \sigma_i^{j-1}) + u_{i-1/2}^{j-1}(\sigma_i^{j-1} - \sigma_{i-1/2}^{j-1/2})],
\end{aligned} \tag{20}$$

then we may derive the fundamental equation

$$\frac{^{n+1}D_i^j - {}^nD_i^j}{\delta t} = -Q_i^j - \Omega^2\Phi_i^j + W_i^j. \tag{21}$$

Finally, we let

$$R_i^j \equiv \frac{^nD_i^j}{\delta t} + Q_i^j - W_i^j, \tag{22}$$

so that the pressure equation to solve is

$$\Omega^2 \Phi_i^j = -R_i^j.$$

Since the procedure for determining the pressures is based on the requirement that ${}^{n+1}D_i^j$ vanish for every cell at the end of the time cycle, we derive the equation for Φ_i^j:

$$\frac{\Phi_{i+1}^j + \Phi_{i-1}^j}{\delta x^2} + \frac{\Phi_i^{j+1} + \Phi_i^{j-1}}{\delta y^2} - \Phi_i^j \left(\frac{2}{\delta x^2} + \frac{2}{\delta y^2}\right) = -R_i^j, \tag{23}$$

or

$$\bar{\Phi}_i^j = \frac{1+\eta}{2\left(\frac{1}{\delta x^2} + \frac{1}{\delta y^2}\right)} \left(\frac{\Phi_{i+1}^j + \bar{\Phi}_{i-1}^j}{\delta x^2} + \frac{\Phi_i^{j+1} + \bar{\Phi}_i^{j-1}}{\delta y^2} + R_i^j\right) - \eta \Phi_i^j, \tag{24}$$

where η is an over-relaxation parameter, and the bar refers to the new iteration value. If Eq. (22) is inserted into Eq. (21), it is seen that ${}^{n+1}D_i^j \equiv 0$ can result from the calculation of the new velocities, provided that the pressure equation is accurately solved. The relaxation of Φ_i^j to its solution occurs through a succession of passes through the mesh. In each pass, the values of Φ_i^j are found from Eq. (24) using the results of the current iteration on those sides where they are available. The convergence criterion that must be satisfied is

$$\left[\frac{|\Phi_{\text{old}} - \Phi_{\text{new}}|}{|\Phi_{\text{old}}| + |\Phi_{\text{new}}| + (v^2)_i^j + (u^2)_i^j + |g_y J \delta y| + |g_x I \delta x|}\right]_{\max} < \epsilon,$$

where $\epsilon = 2 \times 10^{-4}$, or some other suitable small number.

Although $(Q_i^j - W_i^j)$ might have been used instead of R_i^j in Eq. (23), since the two differ in terms proportional to D, the use of R_i^j is more desirable in that the solution of Eq. (23) need not be nearly so accurately derived in keeping the divergence to a low level [14]. This becomes an important consideration, as economy may be gained in computer usage in solving Eq. (24) in the iteration procedure. It should be mentioned, in addition, that the cumulative results of a MAC calculation are independent of whether $(Q_i^j - W_i^j)$ or R_i^j is used in Eq. (23), in the limit of a very stringent ϵ in the convergence criterion.

The basic steps in the solution of a cycle are as follows.

(1) Compute the new values Φ_i^j for all cells, using Eqs. (18), (19), (20), (22), and (24). From these results, φ can also then be found.

(2) Compute the new values of $u_{i-1/2}^j$ and $v_i^{j-1/2}$ in Eqs. (14) and (15), using the new pressures obtained above.

(3) Compute the new turbulence properties through Eqs. (16) and (17), from which σ_i^j and s_i^j can be obtained.

(4) Finally, the marker particles are moved and any necessary bookkeeping is performed to begin the next cycle.

The boundary conditions to be used for a left wall will be discussed for each boundary type, and conditions at other walls are analogous. The indices $(_i^j)$ will refer to the cell inside the system, and $(_{i-1}^{\,j})$ will refer to the imgainary cell outside the system, as shown in Fig. 2. In fact, it is advisable to surround the mesh with "fake" cells, storing the appropriate quantities as shown in Fig. 2, and the program can then automatically compute any functions thereof very simply.

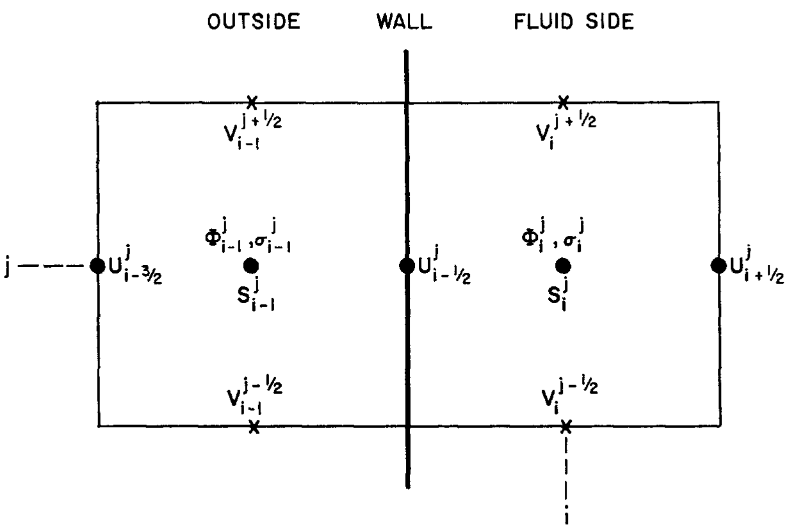

FIG. 2. Field variable positions at a left boundary.

(a) Consider first the case of an input boundary, which allows fluid to move into the system at a given velocity. Here the input velocity, $u_{i-1/2}^j$, along with $\sigma_{i-1/2}^j$ and $s_{i-1/2}^j$, are prescribed.

(1) $u_{i-1/2}^j =$ the prescribed boundary velocity,

(2) $u_{i-3/2}^j = u_{i+1/2}^j$,

(3) $v_{i-1}^{j\pm1/2} = -v_i^{j\pm1/2}$, which forces $v = 0$ on the boundary,

$$(4) \quad \Phi_{i-1}^j = \Phi_i^j - g_x\delta x + \frac{4}{\delta y}(\nu + \sigma_{i-1/2}^j)(v_i^{j+1/2} - v_i^{j-1/2})$$

$$- \frac{\delta x}{\delta y}\left[(\nu + \sigma_{i-1/2}^{j+1/2})\left(\frac{u_{i-1/2}^{j+1} - u_{i-1/2}^j}{\delta y} + \frac{2v_i^{j+1/2}}{\delta x}\right)\right.$$

$$\left. - (\nu + \sigma_{i-1/2}^{j-1/2})\left(\frac{u_{i-1/2}^{j} - u_{i-1/2}^{j-1}}{\delta y} + \frac{2v_i^{j-1/2}}{\delta x}\right)\right],$$

$$(5) \quad s_{i-1}^j = 2(s_{i-1/2}^j) - s_i^j,$$

$$(6) \quad \sigma_{i-1}^j = 2(\sigma_{i-1/2}^j) - \sigma_i^j.$$

(b) The next case considered is that of an output boundary, which allows fluid to leave the system:

$$(1) \quad u_{i-1/2}^j = u_{i+1/2}^j\,;$$

$$(2) \quad u_{i-3/2}^j = u_{i+1/2}^j\,;$$

$$(3) \quad v_{i-1}^{j\pm1/2} = v_i^{j\pm1/2};$$

$$(4) \quad \Phi_{i-1}^j = \Phi_i^j;$$

$$(5) \quad s_{i-1}^j = s_i^j;$$

$$(6) \quad \sigma_{i-1}^j = \sigma_i^j.$$

Note that the above u's, v's, and Φ's have no gradients across the boundary. A linear extrapolation would also be possible for them.

(c) The final possibility we will discuss will be that of rigid walls. A rigid wall may be of either of two types, free-slip or no-slip. A free-slip wall may be considered to represent a plane of symmetry, rather than a true wall, or if the fluid is viscous, a non-adhering or thin-boundary-layer surface. For a free-slip wall, the normal velocity reverses while the tangential velocity remains the same. For a no-slip wall, the tangential velocity also is reversed.

For the *free-slip* wall we have

$$(1) \quad u_{i-1/2}^j = 0,$$

$$(2) \quad u_{i-3/2}^j = -u_{i+1/2}^j\,,$$

$$(3) \quad v_{i-1}^{j\pm1/2} = v_i^{j\pm1/2},$$

$$(4) \quad \Phi_{i-1}^j = \Phi_i^j - g_x\delta x,$$

$$(5) \quad s_{i-1}^j = s_i^j,$$

$$(6) \quad \sigma_{i-1}^j = \sigma_i^j.$$

For the *no-slip* wall we have

(1) $u^j_{i-1/2} = 0,$

(2) $u^j_{i-3/2} = -u^j_{i+1/2},$

(3) $v^{j\pm 1/2}_{i-1} = -v^{j\pm 1/2}_i,$

(4) $\Phi^j_{i-1} = \Phi^j_i - g_x \delta x + \left[\frac{2\nu}{\delta y}(v^{j+1/2}_i - v^{j-1/2}_i)\right],$

(5) $s^j_{i-1} = -s^j_i,$

(6) $\sigma^j_{i-1} = -\sigma^j_i.$

The conditions for s and σ, for both free-slip and no-slip walls, allow for no fluxes of $\mathscr{E}$ or DISS through the wall. As $u^j_{i-1/2} \equiv 0$ at the wall, the convective fluxes are assured to vanish. Also, if the wall is free-slip,

$$\frac{\partial \sigma}{\partial \text{ Normal}} = \frac{\partial s}{\partial \text{ Normal}} = 0,$$

and if the wall is no-slip, then $s = \sigma = 0$ at the wall.

Numerical Stability and Accuracy

The computational stability of the proposed finite-difference equations is affected by several properties of the method.

The first of these relates to the stability of the differential equations themselves. For certain types of problems in which the dynamics imply pressure equilibrium, Eq. (2) shows that $\varphi + 2q/3$ is constant. The diffusion coefficient in Eq. (3) then becomes $\nu + \sigma(\alpha - 2\theta/3\gamma)$, which must be positive. This, of course, implies a consistency requirement on the basic turbulence theory, but it also shows a possible source of numerical trouble for calculations that attempt to explore variations in the universal constants. Equation (4) shows a similar restriction, namely, that $\nu + \sigma(a_3 - 2a_4/3 + a_2)$ be positive in such dynamic-equilibrium flows. For more general flows, these same restrictions would also appear to be necessary.

For stability, the most stringent of the numerical-technique requirements appears to be the one related to diffusion. In addition to the MAC-technique restrictions, it is necessary that

$$2(\nu + a_g \sigma)\, \delta t < \frac{\delta x^2 \delta y^2}{\delta x^2 + \delta y^2},$$

in which a_g is the largest of 1, α, and $a_2 + a_3$. Since σ varies in both space and time, this stability requirement is not fixed, but requires, instead, continual checking and appropriate adjustment of δt.

The time step, δt, can also be seriously limited by accuracy considerations. In regions of strong creation or decay, where the turbulence field variables are changing rapidly, it is necessary for accuracy that the relative change per cycle of q or $\mathscr{D}$ be small. Otherwise the result can easily be an over-shoot of ultimate value, or the occurrence of untenable negative values. For example, in the decay of q, we require

$$\frac{2\nu\Delta}{s^2}\,\delta t \ll 1$$

which may be severely restrictive in regions of small s. (Note the physical interpretation of this restriction, namely, that molecular diffusion must progress in one cycle much less than the distance of one integral scale length, or eddy radius, a completely reasonable requirement.)

The time-step restriction can be relaxed slightly if the transport equations are written (at least in part) in implicit form. Techniques for easing diffusional instability restrictions by implicit formulations are well-known, and could be highly effective here. For creation and decay there is also potential gain. Consider again the decay part of the q equation. In the proposed explicit form,

$$\frac{q^{n+1} - q^n}{\delta t} = -\frac{2\nu\Delta^n q^n}{(s^n)^2},$$

while alternatively we could use q^{n+1} in the term on the right, so that

$$q^{n+1} = \frac{q^n}{1 + \dfrac{2\nu\Delta^n}{(s^n)^2}\,\delta t}.$$

Since the denominator is always positive, the behavior is considerably improved. Generalization to the full q and $\mathscr{D}$ equations therefore prevents one type of large δt catastrophe, namely, the decay to negative values.

In contrast to the stability requirements *added* by the inclusion of turbulence transport, there is one MAC-method stability requirement that is considerably relieved. In MAC calculations, it is necessary that

$$\nu > \text{constant} \times \delta x^2 \frac{du}{dx},$$

in which du/dx is a measure of the maximum velocity gradient and the constant has magnitude of order unity. This restriction is essentially one of molecular Reynolds number, Re, namely,

$$Re \lesssim \left(\frac{D}{\delta x}\right)^2$$

where D is a representative dimension in the flow. With turbulence transport, the condition becomes instead,

$$Re \lesssim \left(\frac{D}{\delta x}\right)^2\left(1 + \frac{\sigma}{\nu}\right).$$

Since σ/ν can be as great as 10^3 or even more, the range of calculable Reynolds numbers is enormously extended.

Discussion

Numerical calculations of fluid flow problems with turbulence are presently impossible unless the turbulence can be represented by some appropriate model. For practical applicability, the model must be relatively simple and capable of coupling with numerical methods for solution of the mean-flow problem.

The numerical-solution technique described in this paper presents one possible approach to the problem that is both broad in scope of applicability, yet minimal in its complexity. Various successful proof-test calculations have been presented elsewhere; the present discussion is designed to contain all the necessary data for preparation of additional computer programs to examine the variety of examples that still need investigation.

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