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A CRITICAL EVALUATION OF UPSTREAM DIFFERENCING APPLIED TO PROBLEMS INVOLVING FLUID FLOW

G.D. RAITHBY

Thermal Engineering Group, Department of Mechanical Engineering, University of Waterloo, Waterloo, Ontario, Canada

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In approximating the convection terms in conservation equations, upstream differences are sometimes used. However, objections, based partly on the appearance of a false or numerical diffusion, are often raised. This paper shows that the false diffusion normally associated with upstream differences is a poor indicator of the total error in approximating the convection terms, and a new definition for false diffusion is proposed. The limiting conditions under which the upstream approximation is valid are then determined; several numerical experiments are performed to determine how much one may depart from these ideal conditions before the upstream approximation leads to unacceptable errors. It is concluded that the upstream approximation is valid only under restricted conditions, but that these include many problems of practical interest.

Introduction

Particularly in the past decade, a very large effort has been expended in developing numerical methods for solving complex multidimensional problems involving fluid flow. Much of this effort has been directed at developing (or sometimes redeveloping) new schemes and methods; comparatively little has been devoted to establishing criteria by which the applicability of the methods to different classes of problems can be judged before their use. The potential user, wishing to "simply" obtain a solution to a problem, is met with a bewildering selection. This paper is intended to provide some of the required insight and practical guidance to make this selection.

The starting point in solutions to these problems is the conservation equations. The term "conservation equations" here refers to the equations expressing conservation of momentum, energy, etc. *together* with the required closure hypotheses relating stress to fluid deformation, conducting to temperature gradient, etc. The first step in early methods was usually to replace derivatives in the differential form of these equations by finite-difference approximations. Central-difference approximations of spatial derivatives, leading to schemes which were "second order", were normally used. For problems involving diffusion alone, or diffusion in a fluid at low Reynolds number, this usually proved satisfactory. However, attempts to obtain high Reynolds number solutions by iterative techniques were often expensive or frustrated by divergence. It was recognized independently by several investigators (e.g. [1, 2]) that less expensive solutions could be obtained by abandoning the central-difference approximation of the convection terms, using instead one-sided (upstream or upwind) differences, and accepting the reduction in the order of accuracy of the scheme to "first order". A large body of literature now exists which condemns this approach (e.g. [3, 4]), but often there is no apparent alternative of reasonable simplicity and economy. Sometimes the resulting solutions clearly do contain unacceptable errors, but in other problems they "look good" or agree well with experiment. For intermediate Reynolds numbers the upstream scheme can be modified [5–8] to blend the advantages of the central and upstream representations.

At present the class of problems for which the upstream approximation of the convective terms can be accurately applied is not well defined. This paper shows that some reasoning has been used incorrectly in the past to condemn the upstream representation, and it proposes guidelines to suggest under what conditions this representation is satisfactory. These conditions are spelled out, wherever possible, in terms of explicit criteria that should be met.

It is concluded that the upstream approximation of convective terms in the conservation equations is not satisfactory for certain classes of problems (or in certain regions within the solution domain), but that in other classes (or other regions) it is both appropriate and highly accurate. The class of problems where its use is justified encompasses many problems of practical interest.

1. The general conservation equation and its discretization

The answers to the problems of interest lie in a determination of density or pressure, velocity, temperature, concentration etc. throughout a region of interest. The fundamental constraints leading to the equations by which these can be determined are the conservation laws. For any conserved, intensive property Φ the conservation equation for any region of volume G with surface area S over the time interval Δt is

$$\underbrace{\int_G [(\rho\Phi)^{t+\Delta t}-(\rho\Phi)^t]\,\mathrm{d}G}_{\mathrm{I}} + \underbrace{\int_t^{t+\Delta t}\int_S \rho\Phi \boldsymbol{V}\cdot\boldsymbol{n}\,\mathrm{d}S\,\mathrm{d}t}_{\mathrm{II}} = \underbrace{\int_t^{t+\Delta t}\int_S \Gamma(\nabla\Phi)\cdot\boldsymbol{n}\,\mathrm{d}S\,\mathrm{d}t}_{\mathrm{III}} + \underbrace{\int_t^{t+\Delta t}\int_G (-\dot{S}\Phi+\dot{P})\,\mathrm{d}G\,\mathrm{d}t}_{\mathrm{IV}}, \tag{1a}$$

where $\boldsymbol{V}$ is velocity, ρ is density, t is time, $\boldsymbol{n}$ is a unit vector normal to the surface of the control volume, Γ is a molecular or effective (molecular plus turbulent) diffusion coefficient, and $-\dot{S}\Phi+\dot{P}$ is a source term. The terms indicate (I) the total increase of Φ within the control volume in time Δt, (II) the net rate at which Φ is transported out of the control volume by convection, (III) the net rate at which Φ enters the control volume by diffusion, and (IV) the source terms for Φ. All terms not explicitly accounted for in I–III are included in IV. The quantity Φ may be specific enthalpy, concentration, specific turbulent kinetic energy etc.; it may be the velocity components themselves (i.e. momentum per unit mass); it may be the vorticity components; or it may be unity (mass per unit mass).

The domain where a numerical solution of one or more of the conservation equations is sought is divided into finite volumes with a nodal point or grid point in each volume. Fig. 1 shows a small section of the domain with a rectangular array of grid points and one volume (dotted lines) surrounding the grid point P. For simplicity Φ has been assumed to depend on only two space dimensions x and y. The volumes are drawn with their surfaces midway between grid points. Grid points surrounding P are designated by upper case symbols, while lower case symbols refer to locations midway between grid points. In finite difference methods rectangular volumes are usual. However, triangular or irregular shaped volumes could also be drawn [9].

The next step is to replace the conservation equation by a set of algebraic equations which involve only values of Φ at the grid points. Several different approaches can be used [10]. For the

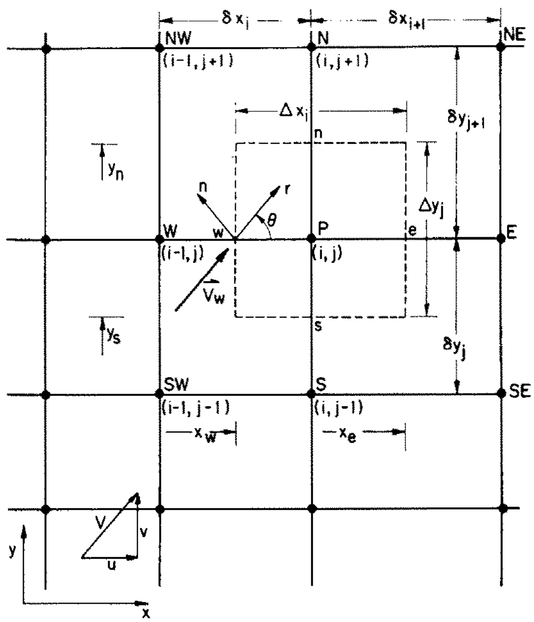

Fig. 1. Grid points, grid lines, and a typical control volume.

present purposes it is useful to describe two of these. The first begins by applying equation (1a) in the immediate vicinity of each grid point over a vanishingly small time interval; this results in the following equation:

I IIa IIb IIIa IIIb IVa IVb

$$\frac{\partial}{\partial t}(\rho\Phi) + \frac{\partial}{\partial x}(\rho u \Phi) + \frac{\partial}{\partial y}(\rho v \Phi) = \frac{\partial}{\partial x}\left(\Gamma \frac{\partial \Phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\Gamma \frac{\partial \Phi}{\partial y}\right) - \dot{S}\Phi + \dot{P}\,, \tag{1b}$$

where u and v are velocities in the x and y directions.

The terms in the equation are approximated at each grid point by replacing the derivatives by finite differences which utilize values of Φ at neighbouring grid points in space and time. The introduction of finite differences in this way is a purely mathematical approximation; when difficulties arise in the solutions, it is difficult to trace these to the underlying violations of physical principles.

Another alternative is to rewrite equation (1a) for the finite volume surrounding each grid point. Thus, for the volume containing P in fig. 1

I IIa IIb

$$[\langle\rho\Phi\rangle^{t+\Delta t} - \langle\rho\Phi\rangle^{t}]\,\Delta x_i\,\Delta y_j + [(\overline{C}_e - \overline{C}_w) + (\overline{C}_n - \overline{C}_s)]\,\Delta t$$

IIIa IIIb IV

$$= [-(\overline{D}_e - \overline{D}_w) - (\overline{D}_n - \overline{D}_s)]\,\Delta t + \overline{\langle(-\dot{S}\Phi + \dot{P})\rangle}\,\Delta x_i\,\Delta y_j\,\Delta t\,, \tag{1c}$$

where

$$\langle\rho\Phi\rangle^t = \int_{y_s}^{y_n} \int_{x_w}^{x_e} (\rho\Phi)^t \, dx \, dy / \Delta x_i \, \Delta y_j \, , \tag{2a}$$

$$\bar{C}_w = \frac{1}{\Delta t} \int_t^{t+\Delta t} C_w \, dt \, , \qquad C_w = \int_{y_s}^{y_n} (\rho u \Phi)_{x_w} \, dy \, , \tag{2b}$$

$$\bar{D}_w = \frac{1}{\Delta t} \int_t^{t+\Delta t} D_w \, dt \, , \qquad D_w = \int_{y_s}^{y_n} \left(-\Gamma \frac{\partial \Phi}{\partial x}\right)_{x_w} dy \qquad \text{etc.} \tag{2c}$$

The numbering on the terms in equation (1c) corresponds to that in equations (1a) and (1b). The quantity C_w is the instantaneous transport of Φ by convection across the w surface of the control volume, while $\bar{C}_w$ is the average flux by this mode over the time Δt. Moreover, D_w refers to the transport by diffusion. Equation (1c) demands the conservation of Φ *on the average* over the volume and over the time interval.

To approximate equation (1c) for each control volume by an algebraic equation requires that the *form* of the profile of Φ between grid points and in time be assumed. The constants in these profile equations are determined using values of Φ at neighbouring grid points and at previous times. These profiles then permit the integrals to be approximated in terms of these Φ values. This method permits the nature of the approximations to be understood and closely monitored. Although the method has much in common with other integral and finite element methods, the resulting algebraic equation is still often referred to as a finite difference equation [10].

It is, of course, often possible to arrive at the same final algebraic equations taking the two different routes. For example, after a number of assumptions to approximate term IIa in eq. (1c), the key one being that Φ varies linearly between W and P and between P and E, one obtains

$$\bar{C}_e - \bar{C}_w \approx \left\{ \rho_e u_e \left[\frac{\Phi_E + \Phi_P}{2}\right] - \rho_w u_w \left[\frac{\Phi_P + \Phi_W}{2}\right] \right\} \Delta y_j \approx \frac{\partial}{\partial x} (\rho u \Phi) \, \Delta x_i \, \Delta y_j \qquad \text{(CAC)} \, , \tag{3}$$

where the Φ's are evaluated at some reference time, say $t + \kappa\Delta t$, in the time interval Δt. The second approximate equality shows that the same result is obtained if term IIa in equation (1b) is replaced by a central difference. Thus, irrespective of the reference time used, this approximation will be called the CAC, standing for the Central Approximation of Convection.

If the linear variation in Φ is replaced by a stepwise variation, where Φ_W is assumed to prevail from W to w, and Φ_P is presumed to prevail from P to e (for $u_w > 0$ and $u_e > 0$), one obtains

$$\bar{C}_e - \bar{C}_w \approx \left\{ \rho_e u_e \Phi_P - \rho_w u_w \Phi_W \right\} \Delta y_j \approx \frac{\partial}{\partial x} (\rho u \Phi) \, \Delta x_i \, \Delta y_j \qquad \text{(UAC)} \, . \tag{4}$$

The second approximate equality shows that the same result would be obtained by replacing term IIa in eq. (1b) by an upstream difference. Irrespective of the time level used in evaluating Φ_P and Φ_W, this will be called the UAC, for Upstream Approximation of Convection.

The material already presented forms the background and framework for the remainder of this paper. The following sections are devoted to an examination and new definition of false diffusion, a discussion of the rationale behind using an UAC, and finally to the results of a series of numerical experiments intended to explore the limitations of the UAC and, to some extent, the CAC.

2. The question of false diffusion

It is on the grounds of a false diffusion argument that the UAC is often abandoned and the virtues of other representations extolled. Therefore a clear resolution of the claims on this subject must be made.

Suppose that the flux of Φ by convection across the w surface of the control volume in fig. 1 is to be estimated. The "number of assumptions" indicated above eq. (3) amount to approximating this flux by $\rho_w u_w \Phi_{w\kappa} \Delta y_j$, where $\Phi_{w\kappa}$ is the exact value of Φ (which would, of course, not be known) at the point w at the time $t+\kappa\Delta t$. Different forms of the spatial interpolation equation used to approximate $\Phi_{w\kappa}$ from values of Φ at surrounding grid points are associated with different schemes (CAC, UAC). It is usual to use a Taylor series to determine the "accuracy" of the approximation; the Taylor series expansions for Φ_W and Φ_P at the time $t+\kappa\Delta t$ (defined as $\Phi_{W\kappa}$ and $\Phi_{P\kappa}$) are

$$\Phi_{W\kappa} = \Phi_{w\kappa} - \left(\frac{\delta x_i}{2}\right)\left(\frac{\partial \Phi}{\partial x}\right)_{w\kappa} + \frac{1}{2!}\left(\frac{\delta x_i}{2}\right)^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_{w\kappa} + \dots , \tag{5a}$$

$$\Phi_{P\kappa} = \Phi_{w\kappa} + \left(\frac{\delta x_i}{2}\right)\left(\frac{\partial \Phi}{\partial x}\right)_{w\kappa} + \frac{1}{2!}\left(\frac{\partial x_i}{2}\right)^2\left(\frac{\partial^2 \Phi}{\partial x^2}\right)_{w\kappa} + \dots . \tag{5b}$$

Suppose that the *approximation* of $\Phi_{w\kappa}$ is called $\phi_{w\kappa}$. According to the UAC, $\phi_{w\kappa} = \Phi_{W\kappa}$. *Neglecting* higher order terms in eq. (5a), the error in the estimate of convected flux due to this approximation is $-\rho_w u_w \Delta y_j (\delta x_i/2)(\partial\Phi/\partial x)_{w\kappa}$. This has the form of a flux of Φ by (false) diffusion with a diffusion coefficient

$$\Gamma^*_{fc,\mathrm{UAC}} = \rho_w u_w (\delta x_i/2) . \tag{6a}$$

The subscript fc is a reminder that this is a False diffusion arising from the estimate of the Convected flux at the instant $t+\kappa\Delta t$ using the UAC.

If a linear profile between W and P is assumed, leading to a CAC, $\phi_{w\kappa} = (\Phi_{W\kappa} + \Phi_{P\kappa})/2$. According to eqs. (5a) and (5b), the coefficient of $(\partial\Phi/\partial x)_{w\kappa}$ in the expression for the error in the approximation of the convected flux is zero; the corresponding false diffusion coefficient is

$$\Gamma^*_{fc,\mathrm{CAC}} = 0 . \tag{6b}$$

It is important to note that the apparent flux by false diffusion across this surface will equal the total error in the estimate of the convected flux (at any instant, due to the error in the assumed spatial distribution of Φ) only when the terms in eqs. (5a) and (5b) of order $(\delta x_i)^2$ and higher are entirely negligible. This will be true if δx_i is small enough.

Often, for reasons of economy, the difference equations must be solved for grid spacings which are either too large or much too large for this to be true. As Roache [11] has pointed out, it then becomes the "size of the error" in the convected flux that concerns us rather than the size or order of the first term in the error expression obtained from a Taylor series.

The approximations involved in estimating the flux of Φ by convection across the w surface are now re-examined by focusing attention on the $\bar{C}_\mathrm{w}$ term in eq. (1c). The definition of $\bar{C}_\mathrm{w}$, and a possible sequence of approximations, is

$$\bar{C}_\mathrm{w}\,\Delta t = \int_t^{t+\Delta t}\int_{y_\mathrm{s}}^{y_\mathrm{n}} (\rho u \Phi)_{x_\mathrm{w}}\,\mathrm{d}y\,\mathrm{d}t \approx \int_t^{t+\Delta t} \rho_\mathrm{w} u_\mathrm{w} \Phi_\mathrm{w}\,\Delta y_j\,\mathrm{d}t\,, \qquad \text{(i)}$$

$$\approx \rho_\mathrm{w} u_\mathrm{w} \Phi_{\mathrm{w}\kappa}\,\Delta y_j\,\Delta t\,, \qquad \text{(ii)} \qquad (7)$$

$$\approx \rho_\mathrm{w} u_\mathrm{w} \phi_{\mathrm{w}\kappa}\,\Delta y_j\,\Delta t = \bar{c}_\mathrm{w}\Delta t\,. \qquad \text{(iii)}$$

Here, as throughout the paper, lower case ϕ's, c's etc. refer to approximations to the corresponding exact values of Φ, C etc. Approximation (i), permitting the integration from y_s to y_n, assumes that $\rho u \Phi$ is constant or varies at most linearly (for a uniform grid spacing) along the w surface. At this stage it is still presumed that Φ_w is known exactly at all times in the Δt interval. Because the temporal distribution is in fact not known, approximation (ii) is made; in this step, Φ_w at the reference time $t + \kappa\Delta t$ (thus the subscript κ, as before) is assumed to prevail over the entire time interval. Approximation (iii) admits that, even at the reference time, $\Phi_{\mathrm{w}\kappa}$ is not known and therefore must be estimated by spatial interpolation between grid points. If only the approximate values ϕ were known at the grid points, not only is the interpolation approximate, but the end points are subject to error. However, these errors are the net *result* of earlier errors (at previous times or iteration levels) in representing all terms in the conservation balance; it is therefore appropriate to exclude this error from eq. (7).

The error in the last two approximations in eq. (7) (due to the unknown temporal and spatial distribution of Φ) can be attributed to a flux by false diffusion as follows:

$$-\Gamma_f \left(\frac{\partial \Phi}{\partial x}\right)_{\mathrm{w}\kappa} \equiv \rho_\mathrm{w} u_\mathrm{w} (\phi_{\mathrm{w}\kappa} - \Phi_{\mathrm{w}\kappa}) + \rho_\mathrm{w} u_\mathrm{w} \left(\Phi_{\mathrm{w}\kappa} - \frac{1}{\Delta t}\int_t^{t+\Delta t} \Phi_\mathrm{w}\,\mathrm{d}t\right). \qquad (8)$$

The remaining approximation in eq. (7) depends on the y distribution of Φ and thus cannot be attributed to false diffusion. Separate diffusion coefficients can be associated with the two terms on the right-hand side of (8) as follows:

$$-\Gamma_{fc} \left(\frac{\partial \Phi}{\partial x}\right)_{\mathrm{w}\kappa} \equiv \rho_\mathrm{w} u_\mathrm{w} (\phi_{\mathrm{w}\kappa} - \Phi_{\mathrm{w}\kappa})\,, \qquad (9)$$

$$-\Gamma_{f\kappa} \left(\frac{\partial \Phi}{\partial x}\right)_{\mathrm{w}\kappa} \equiv \rho_\mathrm{w} u_\mathrm{w} \quad \Phi_{\mathrm{w}\kappa} - \frac{1}{\Delta t}\int_t^{t+\Delta t} \Phi_\mathrm{w}\,\mathrm{d}t \quad . \qquad (10)$$

The diffusion coefficients Γ_{fc} in eq. (9) and Γ^*_{fc} in eq. (6) are closely related since both arise from errors in the assumed distribution of Φ in the x direction. The subscript $f\kappa$ on the diffusion coefficient in (10) serves as a reminder that this apparent flux by False diffusion stems from the assumption that $\Phi_{w\kappa}$ (i.e. Φ_w at $t + \kappa\Delta t$) prevails over the entire time interval. Also, Γ_{fc} and $\Gamma_{f\kappa}$ are additive, i.e.

$$\Gamma_f = \Gamma_{fc} + \Gamma_{f\kappa} \,. \tag{11}$$

Since Γ_{fc} and $\Gamma_{f\kappa}$ may be either positive or negative, so may Γ_f; also, the magnitude of Γ_f may be larger or smaller than the separate magnitudes of Γ_{fc} and $\Gamma_{f\kappa}$, depending on whether the separate errors are additive or partially (or totally) cancel. Note also that as the steady state is approached, $\Gamma_{f\kappa} \to 0$ in eq. (10).

Suppose that the steady state has been reached in a problem involving a variation of Φ in the x direction alone. Then the only error in the estimate of the flux by convection across the w surface is that related to Γ_{fc} in eq. (9) or Γ^*_{fc} in eq. (6). However, $-\Gamma^*_{fc}(\mathrm{d}\Phi/\mathrm{d}x)_{w\kappa}$ is only an *estimate* of the error, while $-\Gamma_{fc}(\mathrm{d}\Phi/\mathrm{d}x)_{w\kappa}$ is equal to the error. If the Φ profile is actually exponential in the x direction, say

$$\Phi = C_1 + C_2 \exp(P_x) \,, \tag{12}$$

where C_1 and C_2 are constants, $P_x = \rho u x/\Gamma$, and $\rho u = \rho_w u_w$ is constant throughout the domain, then the false diffusion coefficients Γ_{fc} for the UAC and CAC can be shown to be

$$\Gamma_{fc,\mathrm{UAC}} = \rho u\, \delta x_i (1 - \exp(-P_\Delta/2))/P_\Delta \,, \tag{13a}$$

$$\Gamma_{fc,\mathrm{CAC}} = -\rho u\, \delta x_i (\cosh(P_\Delta/2) - 1)/P_\Delta \,, \tag{13b}$$

where $P_\Delta = \rho u \delta x_i/\Gamma$ is a grid Peclet number (or grid Reynolds number when Φ is velocity or vorticity since Γ is then viscosity). Equations (6a) and (6b) still define $\Gamma^*_{fc,\mathrm{UAC}}$ and $\Gamma^*_{fc,\mathrm{CAC}}$. When $P_\Delta \ll 1$, the local Φ-profile becomes nearly linear, the higher order terms in the series expansion of Φ rapidly diminish, and the false diffusion coefficients in eq. (13) approach those in (6). However, for $P_\Delta \gg 1$, the two definitions lead to very different results. If one continued to believe that Γ^*_{fc} gives a valid indication of the apparent flux by false diffusion, the CAC would be concluded to be still superior to the UAC. However, eq. (13) would lead to the opposite conclusion ($\Gamma_{fc,\mathrm{UAC}} \to 0$ and $\Gamma_{fc,\mathrm{CAC}} \to -\infty$ as $P_\Delta \to \infty$). The latter conclusion is the correct one; the former is incorrect because it is no longer appropriate to associate the error in the convected flux with the leading term in the Taylor series expression for this error. It is for this reason also that solutions obtained using the UAC sometimes "look good" and compare well with measurements despite an unfavourable Taylor series prognostication.

3. Rationale for choosing upstream and central approximations

One way to guarantee that the results of Taylor series analyses are relevant and accurate is to reduce the grid size and time step to such an extent that, no matter how quickly Φ changes in time or space, these variations are well approximated between grid points by a linear variation. In some problems this may be accomplished with reasonable computer storage and time limitations. However, for many problems of interest, particularly when three space dimensions are involved, this is no longer practical. In these cases alternative guidance must be sought.

From the discussion above it is clear that the total error in the estimate of convected flux is directly dependent on how well the form of the interpolation equations that are used – both in space and time – corresponds to the form of the exact solution under the given conditions. The same is true of the error in approximating other terms. One possibility for better fitting the form of the exact solution would be to assume cubic or quadratic interpolation equations instead of linear ones. Unfortunately, this does not guarantee that the total error will be reduced, and the level of complexity dramatically increases with the order of the equation. If simple equations are to be used with success, it would seem that, for each particular class of problem, (or for sub-domains within the solution domain), the form of these equations should be dictated by the relevant limiting case of the conservation equation.

For example, consider the class of problem (or the region) in which diffusion plays the dominant role in establishing the distribution of Φ. The transport of Φ by diffusion is normal to lines or surfaces of constant Φ; tubes, across whose surfaces there is no flux of Φ, carrying constant and equal fluxes of Φ can be imagined or sketched for any given problem. If the cross-sectional areas of these tubes do not substantially vary over the dimensions of the grid, Φ will decrease almost linearly in the flux direction; then in any other direction Φ also changes linearly (but at a smaller rate). Thus in fig. 1 and eq. (1c) the appropriate profile assumption is that Φ varies linearly between grid points.

If the cross-sectional areas of the tubes carrying Φ do change substantially over the *minimum allowable* grid dimensions, then the linear profile assumption will lead to a poor flux approximation and an inaccurate solution. In this case it is often possible to transform the problem into another coordinate system in which the tube areas do remain approximately uniform; the linear profile assumption will be valid in the new coordinates. This type of coordinate transformation is, in fact, widely and successfully used in numerical modelling. For this diffusion problem see the recent paper by Strong et al. [13].

For problems in which the other terms (besides diffusion) in eq. (1) are not negligible, but still small enough that the *local* distribution of Φ is determined mainly by diffusion, the accuracy of the finite difference representation of the other terms is not particularly important. Even large percentage errors in the fluxes by convection, for example, will still be small compared to the respective total fluxes. However, on the threshold, as convection does begin to play an important role in establishing the spatial distribution of Φ, the linear distribution (central differences) should also be used in estimating the convective flux. As convection effects become still stronger, the Φ profile changes from linear, and neither the fluxes by convection nor those by diffusion are well approximated by the linear profile. Since P_Δ is a measure of the importance of the convective flux relative to the flux by diffusion, for problems in which diffusion and convection play the dominant roles in establishing the distribution of Φ, linear interpolation profiles should be used if $P_\Delta \ll 1$.

As the second example, consider a problem in which convection plays the exclusive role in establishing the distribution of Φ. Applying eq. (1b) over the small region near w in fig. 1 where $\rho \approx \rho_\mathrm{w}$, $u \approx u_\mathrm{w}$ and $v \approx v_\mathrm{w}$,

$$u_w \frac{\partial \Phi}{\partial x} + v_w \frac{\partial \Phi}{\partial y} = V_w \frac{\partial \Phi}{\partial r} = 0 . \tag{14}$$

In this equation r is distance in the flow direction (i.e. in the direction of V_w) measured from w. The solution to this equation is $\Phi = \Phi(n)$, where n is distance measured from w normal to r (see fig. 1). Thus Φ at a given point is established entirely by conditions *upstream*, and the (arbitrary) distribution across the flow is established by boundary conditions. For cases in which the cross-flow variation in Φ can be approximated as linear, the appropriate interpolation equation to use for approximating the convected flux is

$$\phi = C_1 + C_2 n , \tag{15}$$

where C_1 and C_2 are constants to be obtained using values known at grid points which are not downstream of w.

The argument that Φ is established by upstream values is quite simple. If diffusion is not present in the problem, then only first derivatives of Φ with respect to r occur. Thus r/V can be treated as a time-like variable playing exactly the same role as t in the general conservation equation. But any deterministic approach implicitly assumes that Φ at any time depends only on values of Φ at *earlier* times (or on values of Φ upstream in time). Thus, in the absence of diffusion, Φ_w at any r/V depends on values of Φ at smaller r/V, i.e. upstream.

Considering now problems in which convection plays the dominant (but not the exclusive) role in establishing the Φ distribution, the form of the spatial and temporal equations assumed in approximating other terms in eq. (1c) is not very important. However, as diffusion, for example, begins to be important, eq. (15) should be used to estimate the flux by diffusion. For increasingly stronger influences of diffusion, the assumed spatial profile becomes more subject to error, and the estimated fluxes by diffusion and convection both become inaccurate.

When the UAC is used in eq. (1b), it is usual to approximate the diffusion terms IIIa and IIIb by central differences (or linear distributions in eq. (1c)). It is interesting to compare this combination of approximations with those implied in using eq. (15). When $u \to 0$ *or* $v \to 0$, these approximations embody eq. (15) except that diffusion in the flow direction is not zero. This will make little difference for $P_\Delta \gg 1$, but for smaller values (but not "too" near unity) it would be better to drop diffusion entirely in the streamwise direction – if the arguments upon which eq. (15) is based are correct; this point will be examined later in numerical experiments. If both u and v are nonzero (the flow moves at an angle across the grid), the UAC does *not* implicitly embody eq. (15) unless $C_2 \to 0$. Thus, unless the cross-flow gradient in Φ (i.e. C_2) is very small, the use of the UAC, even for $P_\Delta \gg 1$, will lead to significant errors in the flux approximations and therefore in the solution.

4. Restrictions on the upstream approximation of convection

From the discussion above, it appears that the UAC is appropriate when it is the convective terms themselves that are responsible for establishing the distribution of Φ *and* if the flow moves along one of the grid line directions. When other effects (such as diffusion) are present but not important enough to substantially alter the streamwise distributions of Φ, the UAC will still be appropriate. But requiring that other effects be "small" is not very satisfactory; quantitative criteria are needed.

The "other effects" which may affect the accuracy can be easily seen by referring to the general conservation equation. If flow is mainly in the x direction, there are the effects of transients (term I), diffusion in the direction of flow (term IIIa), diffusion across the flow (term IIIb), source terms (terms IVa and IVb), and the convection component in the y direction (term IIb). Criteria are now sought to suggest respectively how fast the transient may be, how large diffusion may become, how large the source terms may be, and how large an angle the flow may make with the grid before the UAC is significantly in error.

Separate criteria are now sought to determine the range of validity of the UAC when each effect *individually* becomes important. When two or more effects simultaneously become important, these criteria will at least provide guidelines for a prospective user. The separate equations to be studied are:

$$\rho u \frac{\mathrm{d}\Phi}{\mathrm{d}x} = \Gamma \frac{\mathrm{d}^2\Phi}{\mathrm{d}x^2} \qquad \text{(problem Ia)}, \tag{16}$$

$$\rho u \frac{\partial \Phi}{\partial x} = \Gamma \frac{\partial^2 \Phi}{\partial y^2} \qquad \text{(problem Ib)}, \tag{17}$$

$$u \frac{\partial \Phi}{\partial x} = -\frac{\partial \Phi}{\partial t} \qquad \text{(problem II)}, \tag{18}$$

$$\rho u \frac{\mathrm{d}\Phi}{\mathrm{d}x} = -\dot{S}\Phi + \dot{P} \qquad \text{(problem III)}, \tag{19}$$

$$u \frac{\partial \Phi}{\partial x} + v \frac{\partial \Phi}{\partial y} = 0 \qquad \text{(problem IV)}. \tag{20}$$

Boundary conditions must also be supplied; these will be chosen to be demanding of the finite difference representations.

To permit a simple analysis of these problems, the usual restriction to constant coefficients is made. In many practical problems, however, the coefficients could depend on space and time and perhaps also directly or indirectly (through other equations) on Φ itself. The conclusions below that are based on the constant coefficient problems give useful guidance for these more complex problems. This is particularly true when the coefficients are "slowly" varying over lengths comparable to the grid dimensions and times comparable to the time step (e.g. if Γ at w and $t + \kappa\Delta t$ adequately represents Γ in the vicinity of w from t to $t + \Delta t$), and the relevant equations are quasi linear, (i.e. values of the coefficients are assumed to be known, at least temporarily, whenever the Φ-equation is operated on). For variable coefficients it is desirable to use the conservative form of the equations [2].

Problem Ia. The effect of diffusion on the UAC: *diffusion in the direction of flow*

Eq. (16) is appropriate in this case, and is rewritten in the following dimensionless form:

$$\frac{d\Phi^*}{dx^*} = \frac{1}{P_L}\frac{d^2\Phi^*}{dx^{*2}}\,, \tag{21a}$$

where Φ has been nondimensionalized such that

$$\Phi^* = 1 \text{ at } x^* = 0\,, \qquad \Phi^* = 0 \text{ at } x^* = 1\,, \tag{21b}$$

$P_L = \rho u L/\Gamma$ is a Peclet number, and L is the reference length $L = x/x^*$. The exact solution to this problem has the form of eq. (12) already discussed. The errors in approximating convection fluxes can be entirely associated with the false diffusion effect in eq. (9) and the false diffusion coefficients in eq. (13).

An *exact* finite difference analog of eq. (21) is now sought. The region $0 \leqslant x^* \leqslant 1$ is divided into $M-1$ equal intervals with spacings $\Delta x^* = 1/(M-1)$; attention is focused on one grid line P (or i) and the control volume surrounding P shown in fig. 1. According to the exact analytical solution to the problem, Φ_P^* is related to the neighbouring values to the east and west (Φ_E^* and Φ_W^*) by

$$\Phi_P^* = A\Phi_E^* + B\Phi_W^*\,, \qquad A = 1/(1+\exp(P_\Delta))\,, \qquad B = 1/(1+\exp(-P_\Delta)) \tag{22}$$

(see appendix A). If this equation can be solved, the exact solution is obtained.

Now a finite difference solution to eq. (21), or its integral counterpart, is sought in which $d\Phi^*/dx$ is approximated by an upstream difference, and in which an "exact finite difference representation" of the diffusion term $d^2\Phi^*/dx^{*2}$ is used. The error in the resulting finite difference solution for ϕ^* can thus be attributed to the UAC alone. The detailed derivation of the finite difference equation is in appendix A; the result is

$$\phi_P^* = a_U\phi_E^* + b_U\phi_W^* \qquad \text{(UAC)}\,. \tag{23}$$

Some explanation of the term "exact finite difference representation", and of attributing the total error to the UAC is necessary. What is meant, as will be seen by reference to appendix A, is that if the approximation of $d\Phi^*/dx^*$ were also exact, then the finite difference solution to the problem would be the exact solution. The upstream-difference approximation of $d\Phi^*/dx^*$, however, is *not* exact, and this results in a direct error in the grid point values of Φ^*. Now because these grid point values are used to determine the fluxes by diffusion, they will also be in error; these result in still additional errors in the grid point estimates of Φ^*. The latter errors are caused indirectly by the former. It seems fair to hold the error in the finite difference approximation of $d\Phi^*/dx^*$ responsible for both. Of course, the indirect errors feed back on the subsequent iteration, for example, to cause additional errors in the convected fluxes (i.e. in the value of $d\phi^*/dx^*$), which again affect the indirect errors and so on. If the errors always reinforce one another with sufficient strength, an iterative solution will be unstable.

Comparing eqs. (22) and (23), we see that a_U and b_U are only approximations of A and B respectively, and it is the errors in these coefficients which drive the solution to ϕ^* away from the exact solution Φ^*. These errors are

$$\delta a_U = a_U - A\,, \tag{24a}$$

$$\delta b_U = b_U - B\,. \tag{24b}$$

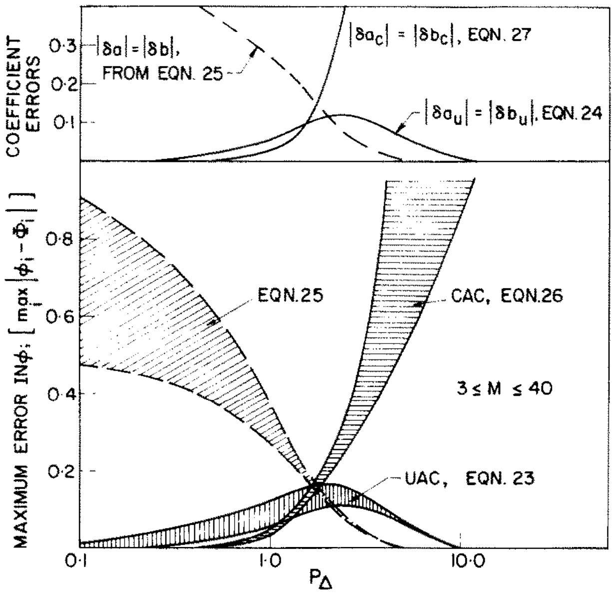

Fig. 2. Errors in coefficients of various finite difference equations (top) and errors in finite difference solutions (bottom) for convection with streamwise diffusion; P_Δ is Peclet number based on the grid spacing Δx.

The magnitudes of these errors are shown in appendix A to depend only on the grid Peclet number $P_\Delta = \rho u \Delta x/\Gamma$. These are plotted in the upper portion of fig. 2. For $P_\Delta \gtrsim 10$ or $P_\Delta \lesssim 0.2$ these errors become negligible. This can be interpreted as implying that the UAC becomes exact at high P_Δ, while at low P_Δ it becomes irrelevant what approximation of convection is used (provided it is somewhat reasonable) because convection is not important in the problem.

Subject to the boundary conditions on this problem, equation (23) was solved for the distribution of ϕ^* for various P_Δ and for various values of grid spacings corresponding to $3 \leqslant M \leqslant 40$. The maximum error in ϕ^* (i.e. $\max_i |\phi_i^* - \Phi_i^*|$, where i is the grid line number) over this range is plotted in the lower portion of fig. 2. The maximum error encountered was about 0.16 at $P_\Delta = 2$; for larger and smaller P_Δ the error decreased. For $P_\Delta \gtrsim 10$ it was negligible.

It was argued previously that when convection is the dominant mode of transport of Φ, eq. (15) would be the most suitable interpolation equation. This amounts to neglecting diffusion in the flow direction altogether in this problem, so that the finite difference equation becomes

$$\phi_P^* = a\phi_E^* + b\phi_W^* \,, \tag{25}$$

where $a = 0$ and $b = 1$. It is verified in this problem (see fig. 2) that the errors in the coefficients a and b are less for $P_\Delta \gtrsim 1.5$, and the maximum error in ϕ^* is also less than with the previous scheme. However, since diffusion is neglected altogether, the error becomes very large at small P_Δ, as suspected previously.

Using a CAC and representing the diffusion term again by an exact finite difference equation one obtains the equation (see appendix A)

$$\phi_P^* = a_C\phi_E^* + b_C\phi_W^* \,. \tag{26}$$

The errors in the coefficients are

$$\delta a_C = a_C - A \,, \tag{27a}$$

$$\delta b_C = b_C - B \,, \tag{27b}$$

and their magnitudes are found to increase very rapidly with P_Δ beyond $P_\Delta \gtrsim 1$ (fig. 2). Eq. (26) was also solved for a large range of P_Δ for $3 \leqslant M \leqslant 40$ using a tridiagonal matrix algorithm [10] (since an iterative solution becomes troublesome for $P_\Delta \gtrsim 2$); the maximum errors in ϕ^* are also shown in fig. 2. Because the CAC is inappropriate at large P_Δ, large errors in ϕ^* result. For $P_\Delta \ll 1$, however, where diffusion dominates in the problem, the CAC is, as expected, superior to the other schemes tested.

It therefore appears that for this problem the UAC is appropriate when $P_\Delta \gtrsim 10$. This is the first of the criteria which are being sought.

Problem Ib. Diffusion normal to the flow direction

We now consider the limitation on the UAC when diffusion normal to the flow becomes important. We write eq. (17) in nondimensional form

$$\frac{\partial \Phi^*}{\partial x^*} = \frac{1}{P_L} \frac{\partial^2 \Phi^*}{\partial y^{*2}} \,, \tag{28a}$$

with the boundary conditions

$$\begin{aligned} \Phi^*(0, y^*) &= 1 \,, \qquad y^* \geqslant 0 \,, \\ \Phi^*(0, y^*) &= 0 \,, \qquad y^* \leqslant 0 \,. \end{aligned} \tag{28b}$$

In this case $P_L = \rho u L/\Gamma$, where Γ is the diffusion coefficient in the y direction. The exact solution to this problem is $\Phi^* = 0.5 + 0.5 \operatorname{erf}(y^* \sqrt{P_L/4x^*})$, where erf is the error function.

A calculation domain $1.0 \leqslant x^* \leqslant 2.0$, $-0.5 \leqslant y^* \leqslant 0.5$ is divided into $M-1$ equal spaces of dimensions Δx^* and Δy^* in the x^* and y^* directions, respectively. Boundary conditions at grid points on the boundary are assigned from the exact solution. For the grid point P (or (i, j)) in fig. 1, one possible form of the exact equation connecting Φ^*_P with the values at the neighbouring grid points is

$$\Phi^*_\mathrm{P} = A_U \Phi^*_\mathrm{W} + C_U \Phi^*_\mathrm{N} + D_U \Phi^*_\mathrm{S} \,, \tag{29}$$

where A_U, C_U and D_U are derived in appendix B.

Now, finite difference solutions to eq. (28) are sought using different approximations of the convection term $\partial \Phi^*/\partial x^*$. An "exact" representation of the diffusion term $\partial^2 \Phi^*/\partial y^{*2}$ is used (cf. remarks after eq. (23) and see appendix B). It should be noted in this case, since diffusion is absent in the flow direction, that eq. (15) would suggest that the UAC is valid for all P_Δ. With the UAC the equation for the approximate solution ϕ^* is

$$\phi_P^* = a_U \phi_W^* + c_U \phi_N^* + d_U \phi_S^* \,. \tag{30}$$

The coefficients a_U, c_U and d_U, which are approximations of A_U, C_U and D_U in eq. (29) have been redefined in this problem, and are listed in appendix B. The errors in these coefficients are

$$\delta a_U = (a_U - A_U)\,, \qquad \delta c_U = (b_U - B_U)\,, \qquad \delta d_U = (c_U - C_U)\,.$$

It is these errors that force the deviation of ϕ^* from the exact solution Φ^*. As a measure of the coefficient errors the maximum values of $|\delta a_U|$, $|\delta c_U|$ and $|\delta d_U|$ are sought throughout the calculation domain. These are plotted in the upper portion of fig. 3 for $M = 11$. The coefficient errors are small for the entire P_Δ range, as expected, with the maximum error occurring at $P_\Delta \approx 20$.

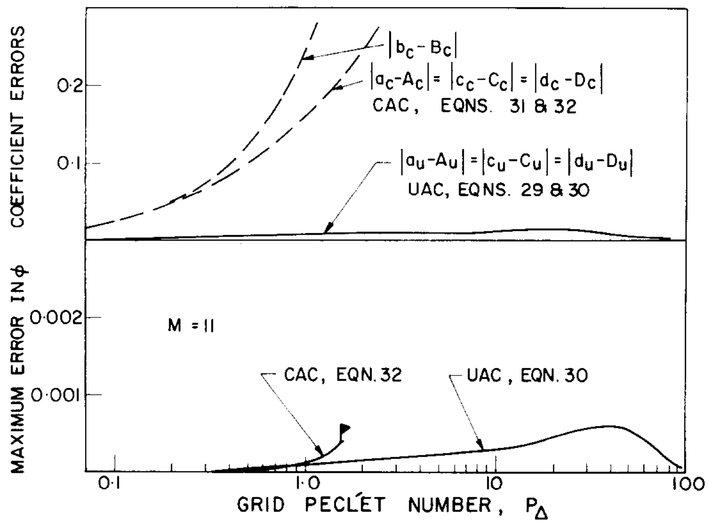

Fig. 3. Errors in coefficients of finite difference equations due to UAC and CAC (top) and errors in finite difference solution (bottom) for convection with cross-flow diffusion; P_Δ is Peclet number based on Δx.

Eq. (30) has also been solved by an iterative procedure and the solution ϕ^* compared with Φ^*, the exact solution. The maximum value of $|\phi_{i,j}^* - \Phi_{i,j}^*|$ across the grid was obtained over a range of P_Δ values for $M = 11$, and the results are plotted in fig. 3. The errors were very small for all P_Δ, reaching a maximum at $P_\Delta \approx 40$.

Now similar results are sought when the CAC is used in eq. (28). The exact solution in this case is rewritten in the form

$$\Phi_P^* = A_C \Phi_W^* + B_C \Phi_E^* + C_C \Phi_N^* + D_C \Phi_S^* \,, \tag{31}$$

where the coefficients are given in appendix B. Replacing $\partial\Phi^*/\partial x^*$ by the CAC and $\partial^2\Phi^*/\partial y^{*2}$ by an "exact" finite difference relation (appendix B), results in

$$\phi_P^* = a_C \phi_W^* + b_C \phi_E^* + c_C \phi_N^* + d_C \phi_S^* \,. \tag{32}$$

The maximum errors in $|\delta a_{CAC}|$, $|\delta b_{CAC}|$ etc. are also plotted in fig. 3. These are seen to be large for $P_\Delta \gtrsim 0.1$. A Jacobi iteration procedure was used to solve eq. (32), subject to exact boundary conditions and with $M = 11$. The maximum value of $|\phi^*_{i,j} - \Phi^*_{i,j}|$ is plotted also in the figure, where it is seen that the error is small for $P_\Delta < 1$ but increases rapidly for $P_\Delta > 1$. Iteration failed to yield a solution for $P_\Delta \gtrsim 1.6$.

From these experiments it can be concluded that the presence of diffusion alone in the cross-flow direction does not seriously affect the accuracy of the UAC, and that this approximation is superior to the CAC for $P_\Delta \gtrless 1$.

Problem II. Transient convection

The accuracy of the UAC will deteriorate if Φ changes with time in the computation domain. The transient effect may arise from boundary conditions which change with time or from a decay of Φ from some initial state towards steady state. The application of the UAC has been previously studied for these problems from several points of view [14, 3, 15], the general conclusion being that the upstream approximation is unsatisfactory. Unfortunately, this has also discouraged the use of the UAC in problems where these conclusions are not relevant.

From the point of view already established above, the transient convection or advection problem (eq. (18)) is now studied, where the transient effects arise from unsteady boundary conditions, and where Φ is convected across the calculation domain in the positive x direction. As the frequency of the boundary disturbance approaches zero, a constant value of Φ prevails over the calculation domain, and the UAC becomes exact. At a higher frequency the UAC becomes subject to error. For given grid-size and time-step restrictions, and for boundary conditions contained within a certain frequency spectrum, the maximum error in Φ in the calculation domain due to the UAC is now sought.

Because of the linear nature of the problem, it is only necessary to study the convection of a single Fourier component across the region. By using superposition, it is then possible to draw conclusions for arbitrary periodic boundary conditions. For simplicity here, the convection of a sine wave of angular frequency ω is studied, leading to the following boundary conditions on eq. (18):

$$\Phi(x, 0) = \sin(-\omega x/u) \,, \quad \Phi(0, t) = \sin(\omega t) \,. \tag{33}$$

The exact solution is then

$$\Phi(x, t) = \sin(\omega t - \omega x/u) \,. \tag{34}$$

A calculation domain is defined in the (x, t)-plane, and this is divided into $M - 1$ equal spaces of dimension Δx in the x direction and into N equal spaces Δt in the t direction. In appendix C an exact finite difference replacement of $\partial\Phi/\partial t$ is derived (note again the remarks after eq. (23)). The derivative $\partial\Phi/\partial x$ is replaced by the UAC, evaluated at the time $t + \kappa\Delta t$. The total error in the approximate solution results, in this case, from the "diffusion-like" errors in eqs. (9) and (10) for which the UAC is responsible. When $\kappa = 0$, $1/2$ and 1, respectively, the resulting finite difference schemes are referred to as (fully) explicit, time centered (Crank–Nicolson) and (fully) implicit. The resulting finite difference equation for the approximate solution ϕ for any κ is

$$\phi_P^{n+1} = a_\kappa \phi_P^n + b_\kappa \phi_W^n + d_\kappa \phi_W^{n+1} , \tag{35}$$

where the subscript κ is a reminder that the coefficients depend on κ, and n corresponds to the time level $n\Delta t$ ($0 \leqslant n \leqslant N$). The coefficients are listed in appendix C.

The exact solution (eq. (34)) can be rewritten in the form of eq. (35) as

$$\Phi_P^{n+1} = A_\kappa \Phi_P^n + B_\kappa \Phi_W^n + D_\kappa \Phi_W^{n+1} , \tag{36}$$

where these coefficients are also given in appendix C. It is the error in the coefficients in eq. (35) which causes ϕ to differ from the exact solution Φ. The coefficients depend on $\omega\Delta t$ and $\omega\Delta x/u$ alone. Because of the number of coefficients, and because each depends on two parameters, it is inconvenient to plot the coefficient errors; however, the maximum errors in ϕ across a grid with $M \geqslant 250$ after $N = 50$ time steps (i.e. the maximum value of $|\phi_i^{50} - \Phi_i^{50}|$, where i numbers the grid lines in the x direction) for $\omega\Delta t = 0.01$, and various $\omega\Delta x/u$ are plotted in fig. 4. The solid circles indicate the errors arising from the explicit scheme ($\kappa = 0$). For $(\omega\Delta x/u) \approx \omega\Delta t$ (or a Courant number of about unity) the maximum error is very small but grows rapidly for $\omega\Delta x/u > \omega\Delta t$, and asymptotically becomes proportional to $\omega\Delta x/u$. For $\omega\Delta x/u < \omega\Delta t$ the scheme becomes unstable (even though the coefficient errors remain small) – this reflects a well known instability.

Similar results for $\kappa = 1/2$ (time-centered) and $\kappa = 1$ are shown in fig. 4. For $\omega\Delta t \ll \omega\Delta x/u$ the errors for all κ are nearly the same. However, the decrease in the error with decreasing $\omega\Delta x/u$ is less rapid as κ increases.

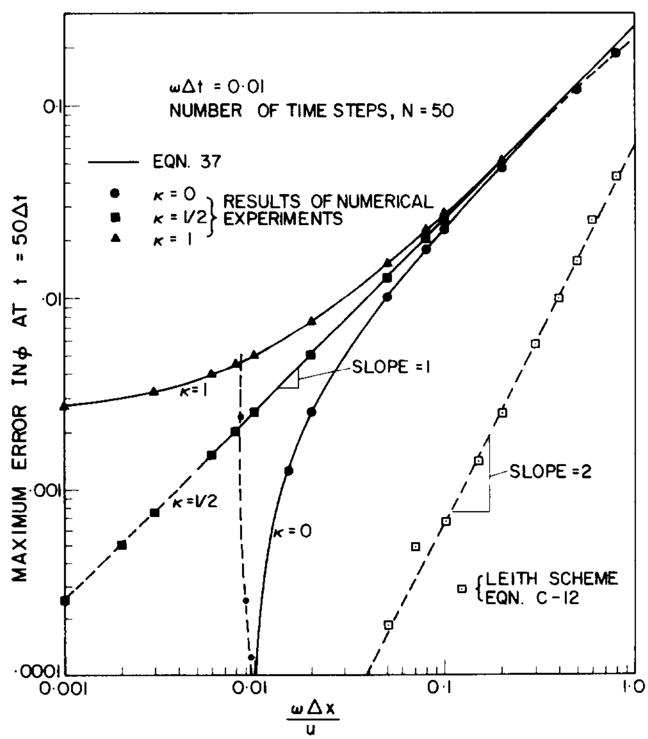

Fig. 4. Errors in finite difference solutions describing convection of a sine wave in x direction after 51 time steps.

This error behaviour can be understood in terms of the "false diffusion" effects discussed earlier. The error in the approximation of the convected flux arises from the two separate errors (from the assumed distribution of Φ in space and time) in eqs. (9) and (10). When $\omega\Delta x/u \gg \omega\Delta t$, almost all of the total error arises from the assumed spatial distribution, or Γ_{fc}, so that the weak dependence of this error on κ, seen in fig. 4, is reasonable. For $\kappa = 1/2$ the error associated with Γ_{fc} remains large compared to that associated with $\Gamma_{f\kappa}$ even for $\omega\Delta t \gtrsim \omega\Delta x/u$; this leads to the linear decrease in the total error with $\omega\Delta x/u$. When $\kappa = 0$ or $\kappa = 1$, the errors associated with Γ_{fc} and $\Gamma_{f\kappa}$ are nearly equal in magnitude for nearly equal values of $\omega\Delta t$ and $\omega\Delta x/u$. However, for $\kappa = 0$ the signs of the errors are opposite, resulting in a cancellation in eq. (11) for Γ_f at $\omega\Delta t \approx \omega\Delta x/u$; for $\omega\Delta t > \omega\Delta x/u$, Γ_f becomes negative and the solution becomes unstable [12]. For $\kappa = 1$ both Γ_{fc} and $\Gamma_{f\kappa}$ have the same sign, resulting in the error remaining large for even small values of $\omega\Delta x/u$; however, because Γ_f remains positive, stability is retained.

For equations of the form of (35), it is possible to obtain a bound for the growth of error in ϕ. Let E^n be the maximum error in ϕ_i^n for $1 < i < M$, then it is shown in appendix C that, when the coefficients in eq. (35) are positive,

$$E^n \lesssim n\{|\delta a_\kappa| + |\delta b_\kappa| + |\delta d_\kappa|\}/(1 - |D_\kappa|)\,, \qquad \delta a_\kappa = a_\kappa - A_\kappa \text{ etc.} \tag{37}$$

This equation is plotted in fig. 4 for comparison with the results of the numerical experiments described above. It can be seen that the approximate upper bound given by this equation is in excellent agreement with the maximum errors found in the numerical experiments.

So far the magnitude of the errors in ϕ have not been discussed. Reference to fig. 4 shows that these can be large. After only 50 time steps the maximum error in ϕ (which appears as a damping of the sine wave) is about $2\frac{1}{2}$ percent of the amplitude for $\omega\Delta x/u = 0.1$ and $\omega\Delta t = 0.01$. Another undesirable feature is the nearly linear dependence of the error on N *and* Δt for a given value of $\omega\Delta x/u$. If a better accuracy were sought by decreasing Δt, the total number of time steps N required to reach a given real time would also increase in such a way that very little increase in accuracy would be achieved. Thus, the application of the UAC is limited to cases where ω is small.

Conclusions can now be drawn for the convection of an arbitrary boundary distrubance, represented by the sum of its Fourier components, across the domain. Using an UAC, the estimate of the error in the individual components is now known (eq. (37)), so that an estimate of the total error can be obtained by adding the errors in the individual Fourier components weighted by the Fourier coefficients from the series representation of the boundary disturbance. The result is that all but the very low frequency components suffer a large error (damping for stable schemes), the error increasing as the scheme becomes more implicit (κ increases).

It is appropriate here to enquire why the UAC is not satisfactory, except at such low frequencies, for transient convection. The rationale behind the UAC was that the conservation equation demanded that the upstream values of Φ should prevail downstream when convection alone dominates. However, in the presence of the transient terms the same equation does *not* demand that $\Phi(x, t)$ become even approximately constant in the flow direction unless the frequency is so low that boundary values of Φ are carried almost unchanged along streamlines across the calculation domain.

When transient convection does dominate in determining the spatial and temporal distribution of Φ in the calculation domain, the conservation equation demands rather that $\Phi(\boldsymbol{r}, t + \Delta t) \approx \Phi(\boldsymbol{r} - \boldsymbol{V}\Delta t, t)$ for a region of uniform velocity, $\boldsymbol{V}$. The finite difference scheme used should embody (or perhaps be constructed upon) this constraint as Leith [16] has done. The conservation equation provides no guidance on the form of interpolation equations (linear, quadratic etc.) to be used in the flow direction; this will depend on how Φ at the boundary is changing with time. Linear interpolations would be used if Φ was adequately represented by piecewise linear equations over the time steps and grid spaces used. If Φ changed with time in a highly nonlinear fashion at the boundary, exponentially perhaps, then the appropriate interpolation equation in space would be exponential in the flow direction and perhaps linear normal to the flow direction.

The present problem of transient convection of a sine wave in the x direction was also solved using a modified Leith scheme (modified in the sense that $\partial\Phi/\partial t$ was replaced with an "exact" finite difference expression). This equation is derived in appendix C. The maximum error in ϕ for $\omega\Delta t = 0.01$ for a range of $\omega\Delta x/u$ is shown in fig. 4; the errors are one to two orders of magnitude lower than those obtained previously using the UAC.

To summarize the results of this section, for a simple one-dimensional convection of boundary disturbances across a calculation domain the UAC leads to large errors for all but the very low frequency components. Thus, for problems in which transients and convection are both important, the use of the UAC should be restricted to those problems in which (a) the transient solution itself is not of interest but only a means to reaching a steady-state solution, or (b) the maximum frequency of interest is very low. The latter case requires (see text above) that transients be so slow that the solution to the problem at any instant be nearly the same as the steady-state solution subject to the boundary conditions at that instant.

Some additional observations are also appropriate. The above results have been obtained in the total absence of real diffusion, the idea being that the influence of transients, diffusion, and source terms on the accuracy of the UAC would be tested separately. If both diffusion and transients were simultaneously important, one could argue that real diffusion is sometimes large enough to mask the false diffusion arising from the approximation of the transient convection terms. This may be true in certain problems or in certain sundomains in problems, but care must be exercised that diffusion is not so dominant that the $P_\Delta \gtrsim 10$ criterion of the previous section is violated.

Problem III. The effect of source terms on the UAC

When the transient and diffusion terms vanish from the general conservation equation and the source terms remain, eq. (19) results. We wish to determine how large $\dot{S}$ and $\dot{P}$ may become before these terms threaten the dominance of convection in determining the streamwise Φ profile and therefore destroy the accuracy of the UAC.

Assuming that in the region of interest ρ, u, $\dot{S}$ and $\dot{P}$ are constant (or locally nearly constant), eq. (19) becomes, in nondimensional form,

$$\frac{1}{\dot{S}_L^*}\frac{\mathrm{d}\Phi^*}{\mathrm{d}x^*} = -\Phi^* + 1\,. \tag{38a}$$

The boundary condition

$$\Phi^*(0) = 0 \tag{38b}$$

is specified. Here $x^* = x/L$, where L is any reference length, $\dot{S}_L^* = (\dot{S}L/\rho u)$ and $\Phi^* = \Phi/(\dot{P}/\dot{S})$. For $\dot{S}_L^* > 0$, Φ^* asymptotically approaches unity, while for $\dot{S}^* < 0$, Φ^* grows exponentially without limit. In particular, $\dot{S}_L^* = 0$ is a special case in which the above nondimensionalization is inappropriate. When $\dot{S} = 0$ in eq. (19), it is seen that Φ grows linearly with x.

This problem is now analysed as in the previous cases. Representing convection by the UAC results in the equation

$$\phi_P^* = a_U \phi_W^* + b_U \ , \tag{39}$$

where, in this problem, $a_U = 1/(1 + \dot{S}_\Delta^*)$ and $b_U = \dot{S}_\Delta^* a_U$, and where $\dot{S}_\Delta^* = \dot{S}\Delta x/\rho u$. The exact solution in the form of eq. (39) is

$$\Phi_P^* = A_U \Phi_W^* + B_U \tag{40}$$

where $A_U = \exp(-\dot{S}_\Delta^*)$ and $B_U = (1 - A_{UAC})$.

Comparing coefficients as before, we see that the UAC leads to accurate coefficients in the two extremes as $\dot{S}_\Delta^* \to 0$ and $\dot{S}_\Delta^* \to +\infty$. For $\dot{S}_\Delta^* < 0$, the coefficients are in large error except for $|\dot{S}_\Delta^*| \ll 1$. The calculated maximum errors in Φ^* for 10 and 20 grid lines, respectively, in the x^* direction are shown in fig. 5. The explosive growth of the error for $\dot{S}_\Delta^* < 0$ is clearly demonstrated. For $\dot{S}_\Delta^* > 0$, to obtain a solution accurate to 1 percent required that $\dot{S}_\Delta^*$ be less than 0.05.

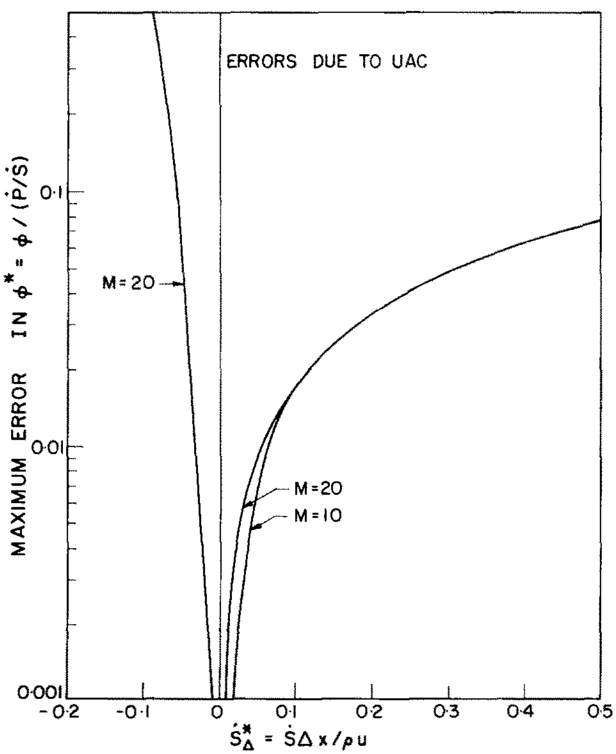

Fig. 5. Errors in solution of convection problem with source terms of form $-\dot{S}\Phi + \dot{P}$.

As $\dot{S}^*_\Delta \to 0$, the error in ϕ^* also rapidly diminishes. In this limit the coefficients become exact. Although ϕ^* is not an appropriate variable for $\dot{S}^*_\Delta = 0$, this result implies that $\phi \to \Phi$ as $\dot{S} \to 0$ for a constant $\dot{P}$ value.

Problem IV. Convection at an angle to the grid lines

So far the velocity convecting Φ has been assumed to be along a grid line direction (x direction) so that term IIb vanished in eqs. (1b) and (1c). When both velocity components u and v are non-zero, the problem becomes either quasi-two-dimensional or fully two-dimensional. Quasi-two-dimensionality is defined here as a two-dimensional dependence of Φ which can be reduced to a one-dimensional dependence by rotating the x–y coordinate system. The problems already considered of convection in balance with *streamwise* diffusion, with transient storage and with source terms, all have quasi-two-dimensional counterparts. In each of these cases Φ is constant in the cross-flow direction (n direction in fig. 1). By numerical experiments and analysis the author has found that in each of these cases the UAC leads to *more* accurate results than when the flow moves along a grid line direction. For equal grid spacing in the x and y directions the minimum errors occurred with $u = v$. This can be seen by noting that, as θ in fig. 1 increases from 0° to 90°, the error in the convected flux through the w face *decreases* monotonically to zero (for these problems). On the other hand, the error in the flux through the s face *increases* monotonically with θ. The minimum error in the total flux into the control volume through the w and s surfaces occurs at 45° for the $\Delta x = \Delta y$ grid.

Fig. 6 shows, as an example, the maximum error which occurs when a sine wave variation in Φ is convected at various angles across a square calculation domain with $\Delta x = \Delta y$. The solid curve is an approximate upper bound on the error from an analysis similar to that used to obtain eq. (37). The solid symbols were obtained from numerical experiments.

For fully two-dimensional problems there are variations in Φ in the streamwise *and* cross-flow directions. If convection is responsible for establishing the streamwise distribution of Φ, eq. (15) becomes an appropriate interpolation equation for estimating the convected flux of Φ across control volume surfaces. The UAC does not embody this type of interpolation unless C_2 is zero (i.e unless the problem *is* quasi-two-dimensional). Thus, when cross-flow variations of Φ are large, the UAC is expected to be in substantial error. This has already been discussed by Gosman et al. [17] and by de Vahl Davis and Mallinson [18].

To demonstrate the errors which arise from the failure of the UAC to properly estimate convective fluxes in the presence of strong cross-flow gradients in Φ *and* when the flow cuts across the grid at an angle, some numerical experiments on the solution of eq. (20) are reported. This equation is rewritten in the form

$$u^* \frac{\partial \Phi^*}{\partial x^*} + v^* \frac{\partial \Phi^*}{\partial y^*} = 0 , \tag{41}$$

where $u^* = u/V$, $v^* = v/V$, $x^* = x/L$, $y^* = y/L$, $V = (u^2 + v^2)^{1/2}$, and L is the side of the square (see fig. 7) in which the equation was solved. The boundary conditions specify a step change in Φ^* normal to the flow direction from $\Phi^* = 1$ to $\Phi^* = 0$ as shown in fig. 7. Using the UAC, finite difference solutions to eq. (41) were sought for various grid spacings and for the flow cutting across the grid at various angles θ from the x^* direction. The finite difference calculation of ϕ^*

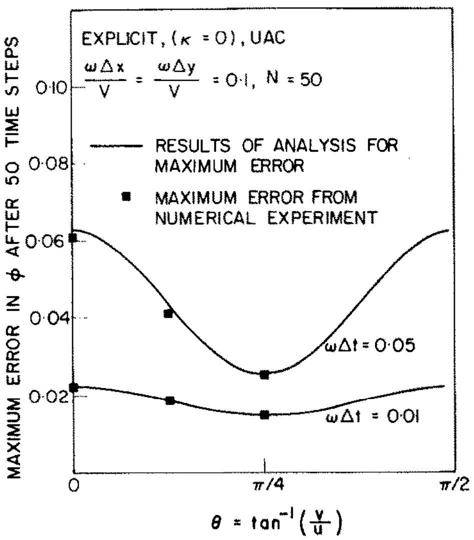

Fig. 6. Error in finite difference solution describing convection of a sine wave at various angles across a two-dimensional region after 50 time steps. Amplitude of sine wave is unity.

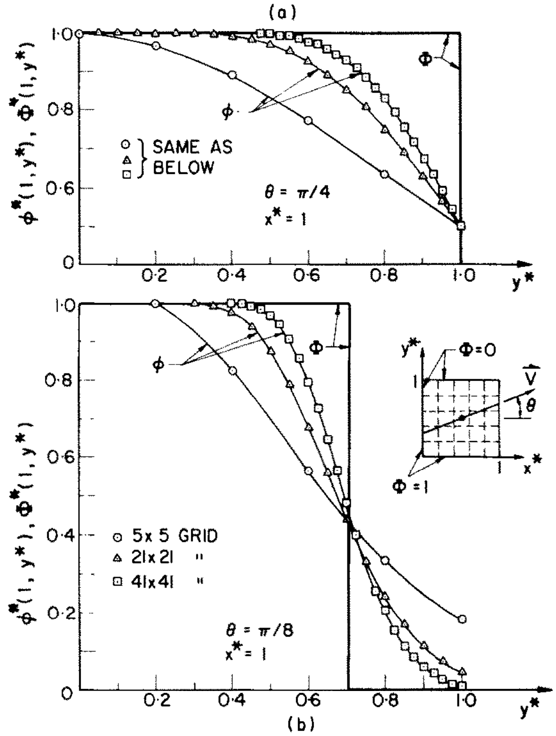

Fig. 7. Numerical experiments of convection across square region shown in insert; ϕ and Φ are finite difference and exact solutions, respectively.

on $x^* = 1$ is shown in fig. 7 for $\theta = \pi/8$ and $\theta = \pi/4$. The exact solution Φ^*, which simply maintains the step shape of the profile across the calculation domain, has been shown for comparison.

When $\theta \neq 0$ or $\theta \neq \pi/2$, the error in the convected fluxes, associated partly with eq. (9), results in an apparent (false) diffusion of Φ normal to the flow direction. This apparent diffusion depends on θ and is maximum, as will be seen, at $\theta = \pi/4$. Reducing the grid size at a given θ reduces this apparent diffusion (see fig. 7), but an extremely fine grid would be required to closely maintain the shape of the step change across the domain.

A cross-flow gradient as sharp as that in the preceding calculation is rarely found in practice. (except at shock waves). Usually this gradient would be such that, over typical grid dimensions, Φ could be approximated as linear in the cross-flow direction, i.e. eq. (15) would be valid. For such a distribution the exact convected flux of Φ across the w surface of the control volume in fig. 1 would be (assuming steady state)

$$C_w = \rho_w u_w \Delta y_j C_1 . \tag{41}$$

According to the UAC, for $u_w > 0$ the value of ϕ_w is estimated by $\Phi_W = C_1 - C_2(\delta x_i/2)\sin\theta$ where δx_i and θ are defined in fig. 1. The estimated flux by convection c_w is therefore

$$c_w = C_w - (\tfrac{1}{4}\rho_w V_w \Delta y_j \delta x_i \sin 2\theta) C_2 . \tag{42}$$

The error $c_w - C_w$ has the features seen above in the numerical experiments. If the flow is along one of the grid line directions, $\sin(2\theta) = 0$, so that the error vanishes. It also vanishes for $\sin(2\theta) \neq 0$ if the cross-flow gradient in Φ is small, i.e. $C_2 = (\partial\Phi/\partial n)_w \to 0$. When C_2 is large, the maximum error occurs at $\theta = \pi/4$.

Eq. (42) can be used to obtain a criterion on what combinations of cross-flow gradient and angle of flow to the grid line direction are permissible. If, in subdomains of the solution domain, it is required that the error in the estimate of the convected flux across any surface be small compared to the maximum flux that could occur across the surface, then the following condition must be satisfied

$$\left\{\frac{\partial\Phi}{\partial n}\,|\sin 2\theta|\right\}_{\mathrm{MAX}} \ll 4\left\{\frac{|\Phi|}{\Delta x}, \frac{|\Phi|}{\Delta y}\right\}_{\mathrm{MAX}}, \tag{43}$$

where the subscript MAX refers to the maximum value of the quantity or quantities in parenthesis within the subdomain. Applying this criterion to the entire solution domain may result in unjustifiably stringent conditions.

In the section on Transient Convection it was observed that it might be possible to accept large errors in the UAC provided that these errors were sufficiently masked by the real diffusion within the flow. This may also be applied here as an alternative to satisfying equation (43). de Vahl Davis and Mallinson [18] have shown that the apparent or false diffusion coefficient arising from the use of the UAC when flow cuts across a grid at an angle is given approximately by

$$\Gamma_f = \frac{V\Delta x\,\Delta y \sin(2\theta)}{4[\Delta y \sin^3\theta + \Delta x \cos^3\theta]}\,. \tag{44}$$

This result was reported to agree well with a similar expression by Wolfstein [17] based on numerical experiments. Thus, the false diffusion effect will be masked by real diffusion if $\Gamma_f \ll \Gamma$. This condition could often be satisfied in low-velocity laminar flow or in turbulent flow where Γ is large. This is often argued (see [17] for example). However, as in the previous case, large errors from the UAC may be expected if Γ is so large that $P_\Delta < 10$.

In conclusion to this section, it is appropriate to observe that the questions relating to the applicability of the UAC to problems where the flow cuts across the grid are not entirely resolved. If, as stated above, $\Gamma_f \ll \Gamma$ but still $P_\Delta \gtrsim 10$, the errors in the UAC are masked by real diffusion (Γ_f is calculated from (44)). However, if as is often the case, $\Gamma_f \gtrsim \Gamma$ or $\Gamma_f \gg \Gamma$, we do not know whether the UAC is accurate or not; this depends on the magnitude of the cross-flow gradients in Φ. One is then forced back to the use of eq. (43). But now experience is lacking on what numerical value should be attached to the inequality, and on how large the subdomains should be. Also, even if these questions were answered, how should one proceed if the inequality were not satisfied?

The latter problem has been now partly resolved by introducing new differencing schemes which embody eq. (15). This is the topic of a separate study [19].

5. Summary of results

In reducing a partial differential or an integral equation expressing conservation of Φ to an algebraic equation, it is necessary to approximate the convected flux of Φ. A Taylor series shows that an upstream approximation of the convected flux has a false diffusion associated with it. A false diffusion arising out of such an analysis is shown to be sometimes a poor indicator of the total error in the estimate of convected fluxes. Under certain circumstances an upstream approximation of convected fluxes becomes highly accurate, and the usual definition of false diffusion becomes inappropriate.

The rationale behind using an upstream approximation of convection indicates that its use is appropriate when

(1) steady or nearly steady convection plays the dominant role in establishing the spatial distribution of the transported quantity Φ, and

(2) *either* the flow is closely aligned with grid lines (quasi-one-dimensional problem) *or* there are no strong cross-flow gradients in Φ.

A systematic study was then undertaken to determine how large "other effects" could become before the accuracy of the upstream approximation became significantly (and adversely) affected. The "other effects" considered were those influencing (1) and (2) in the previous paragraph; the effects considered to challenge the role of convection in establishing the spatial distribution of Φ (i.e. condition (1)) were diffusion, transients, and the presence of sources or sinks for Φ. For the upstream approximation of convection to be accurate, it was found to be necessary that the following conditions be satisfied:

(1) For problems in which flow moves along grid lines

(a) In the presence of diffusion, it is necessary that the grid Peclet number P_Δ (based on the grid dimension in the flow direction) be of order 10 or larger.

(b) In the presence of transients, large errors result in the use of the upstream approximation for all but very small frequencies (or for all Fourier components except those of low wave number).

(c) In the presence of source terms of the form $-\dot{S}\Phi + \dot{P}$, large errors result unless $\dot{S}$ is small. The numerical experiments suggest that, for high accuracy, $-0.03 < \dot{S}\Delta/\rho V \leqslant 0.05$ should be satisfied, where Δ is the grid dimension in the flow direction, and V is the velocity. When this parameter is larger than 0.05, the increase in the error is modest. However, larger negative values result in a rapid escalation of the error. When $\dot{S} = 0$, the error due to the $\dot{P}$ term alone is small, at least provided that $\dot{P}$ is nearly uniform across the grid.

(2) For problems in which flow does not move along grid lines

(a) In the absence of cross-flow gradients in Φ, the upstream approximation of advection is more accurate than when the flow moves in a grid line direction.

(b) In the presence of cross-flow gradients in Φ, the accuracy to which the upstream approximation estimates the convective fluxes is reduced. Thus, the justification for a continued use of the upstream approximation in this case requires that either

(i) the combination of the angle of flow across the grid and the cross-flow gradient in Φ must be such that eq. (43) is satisfied, or

(ii) the errors in estimating fluxes by convection, which appear as apparent or numerical diffusion, must be small enough that the numerical or false diffusion is small compared with real diffusion.

Acknowledgements

The conclusions drawn in this manuscript are the results of many small and separate investigations and numerical experiments conducted over the past several years. Discussions with Drs. S.V. Patankar, formerly of this University, and K.E. Torrance of Cornell University have been very helpful. Dr. B. Simpson, also of this University, suggested the simple error-bound analysis in section (b) of appendix C after many earlier attempts by the author to obtain error bounds at each grid point and each time level had bogged down in complexity.

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Appendix A. The effect of streamwise diffusion on the UAC

A finite difference solution to eq. (21), or rather its integral equation counterpart, is sought in the domain $0 \leqslant x^* \leqslant 1$ using the grid line system described in the text. The object is to find the the errors in this solution which result from the UAC. However, if one approximates convection using an UAC and diffusion by some other approximation, the error in the resulting solutions is due to *both* these approximations. What is needed is an exact representation for the diffusional flux in the sense that if the convection approximation becomes exact, the solution becomes exact.

Recognizing that Φ^* is uniform in the y direction and invariant with time, we integrate eq. (21) over the control volume surrounding P in fig. 1; the grid spacing is presumed uniform. The equation becomes

$$\Phi^*_e - \Phi^*_w = \frac{1}{P_L}\left[\left(\frac{d\Phi^*}{dx^*}\right)_e - \left(\frac{\partial\Phi^*}{dx^*}\right)_w\right]. \tag{A.1}$$

Since, for this problem, Φ^*_e lies between Φ^*_P and Φ^*_E, one can write [7]

$$\Phi^*_e = (\tfrac{1}{2} + \alpha_e)\Phi^*_P + (\tfrac{1}{2} - \alpha_e)\Phi^*_E\,, \qquad |\alpha_e| \leqslant 1/2\,, \tag{A.2a}$$

$$\left(\frac{d\Phi^*}{dx^*}\right)_e = \gamma_e\left\{\frac{\phi^*_E - \Phi^*_P}{\Delta x}\right\}. \tag{A.2b}$$

Similar expressions can also be written for the w surface. A wide variety of differencing schemes can be generated by choosing different values of the "weighting factors" α_e, γ_e etc. The exactly correct values of these *may* be different for each surface of the control volumes. These exact values can be found by substituting the exact (analytical) solution to the problem into (A.2a) and (A.2b) and solving for α_e and γ_e. By analogy, α_w and γ_w can then be written down. In this problem it turns out that $\alpha_e = \alpha_w = \alpha$ and $\gamma_e = \gamma_w = \gamma$. The resulting expressions for α and γ are given later. With α and γ known, the relations between Φ^*_e, $(d\Phi^*/dx^*)_e$ etc. and the grid point values are exactly known. Eqs. (A.2a) and (A.2b), along with similar equations for the w face, are substituted back into (A.1), thereby obtaining the following exact relationship between the values of Φ^* at the three grid points W, P and E:

$$\Phi_P^* = \left(\tfrac{1}{2} - \frac{1/4}{\alpha + \gamma/P_\Delta}\right)\Phi_E^* + \left(\tfrac{1}{2} + \frac{1/4}{\alpha + \gamma/P_\Delta}\right)\Phi_W^* \ . \tag{A.3}$$

The quantities in parentheses are the coefficients in eq. (22).

If the exact solutions were not known, then various flux approximations would be equivalent to choosing different approximations of α and γ. Call these approximate values $\tilde{\alpha}$ and $\tilde{\gamma}$ respectively; then the finite difference equation for ϕ^* becomes

$$\phi_P^* = \left(\tfrac{1}{2} - \frac{1/4}{\tilde{\alpha} + \tilde{\gamma}/P_\Delta}\right)\phi_E^* + \left(\tfrac{1}{2} + \frac{1/4}{\tilde{\alpha} + \tilde{\gamma}/P_\Delta}\right)\phi_W^* \ . \tag{A.4}$$

An UAC for $u > 0$ is obtained by setting $\tilde{\alpha} = 1/2$, while the CAC is equivalent to $\tilde{\alpha} = 0$. A central difference approximation of the diffusion term is equivalent to setting $\tilde{\gamma} = 1$. The object here is to find the error in ϕ_P^* due to the error in $\tilde{\alpha}$ alone. Thus $\tilde{\gamma}$ is set equal to γ in eq. (A.4), and ϕ_P^* is obtained by using respectively values of $\tilde{\alpha} = 0$ for the CAC and $\tilde{\alpha} = \frac{1}{2}$ for the UAC. In accordance with the remarks in the paragraph following eq. (23), the error in ϕ_P^* which results can be attributed to the approximation of the convection terms alone.

Therefore, A and B in eq. (22) are equated to the coefficients in eq. (A.3), a_U and b_U in (23) are obtained from (A.4) with $\tilde{\alpha} = 1/2$ and $\tilde{\gamma} = \gamma$, and a_C and b_C in (26) are obtained from (A.4) with $\tilde{\alpha} = 0$ and $\tilde{\gamma} = \gamma$.

By the method described above, knowing that the exact solution to the problem has the form of eq. (12), one can show [7] that

$$\alpha = 0.5 - [\exp(P_\Delta/2) - 1]/[\exp(P_\Delta) - 1] \ , \qquad \gamma = P_\Delta \exp(P_\Delta/2)/[\exp(P_\Delta) - 1] \ .$$

After some algebraic manipulation the substitution of these expressions into the coefficients into eq. (A.3) gives the equations for A and B in eq. (22).

Appendix B. Diffusion normal to flow direction

The integral equation counterpart of eq. (28) over the volume in fig. 1 surrounding P is

$$\int_{y_s}^{y_n} (\Phi)_{x_e}\, dy - \int_{y_s}^{y_n} (\Phi)_{x_w}\, dy = \frac{1}{P_L}\left\{\int_{x_w}^{x_e} \left(\frac{\partial\Phi}{\partial y}\right)_{y_n} dx - \int_{x_w}^{x_e} \left(\frac{\partial\Phi}{\partial y}\right)_{y_s} dx\right\} , \tag{B.1}$$

where the stars denoting dimensionless quantities have been dropped. Following the procedure outlined above, assuming that the grid spacings in the x and y directions are uniform, results in

$$\frac{1}{\Delta y}\int_{y_s}^{y_n} (\Phi)_{x_e}\, dy = (\tfrac{1}{2} + \alpha_e)\Phi_P + (\tfrac{1}{2} - \alpha_e)\Phi_E \ , \tag{B.2a}$$

$$\frac{1}{\Delta x}\int_{x_w}^{x_e} \left(\frac{\partial\Phi}{\partial y}\right)_{y_n} dx = \delta_n\left(\frac{\Phi_N - \Phi_P}{\Delta y}\right) \qquad \text{etc.} \tag{B.2b}$$

The exact solution is known (see text), so that α_e, α_w, δ_n and δ_s can be found for each grid point from these equations. Note that, because of symmetry about the surfaces of the control volume, α_e for the volume centered at P is equal to α_w for the volume centered at E, δ_n for the volume centered at P equals δ_s for the volume centered at N etc.

The "exact" equation connecting Φ_P with its neighbouring points is then

$$\Phi_P = \left\{\frac{(\frac{1}{2} + \alpha_e)}{F}\right\} \Phi_W + \left\{\frac{(\alpha_w - \frac{1}{2})}{F}\right\} \Phi_E + \left\{\frac{\delta_n \Delta x}{F P_L \Delta y^2}\right\} \Phi_N + \left\{\frac{\delta_s \Delta x}{F P_L \Delta y^2}\right\} \Phi_S\,, \tag{B.3}$$

where $F = (\alpha_e + \alpha_w) + (\delta_n + \delta_s)\,\Delta x/P_L\,\Delta y^2$.

The coefficients A_C, B_C, C_C and D_C in eq. (31) are associated respectively with the coefficients in eq. (B.3) from left to right. The approximate coefficients in eq. (32) are obtained by replacing α_e and α_w in the exact coefficients by $\tilde{\alpha}_e = \tilde{\alpha}_w = 0$. It should be noted that, even when exact coefficients are used, as in (B.3), an *iterative* solution cannot always be used to solve for the Φ_P. However, when the exact solution is substituted into eq. (B.3), the equation is satisfied exactly.

The form of eq. (B.3) can be converted to the form of the equation which arises when an UAC is used (i.e. eqs. (29) and (30)). This requires that Φ_E be removed from the equation using

$$\Phi_E = g\Phi_P + f\Phi_W\,. \tag{B.4a}$$

The exact solution $\Phi = \frac{1}{2} + \frac{1}{2}\,\mathrm{erf}\,(\eta)$, where $\eta = (y\sqrt{P_L/4x})$, gives the following constraints for g and f:

$$g = \frac{\mathrm{erf}\,(\eta_E) - \mathrm{erf}\,(\eta_W)}{\mathrm{erf}\,(\eta_P) - \mathrm{erf}\,(\eta_W)}\,, \qquad f = 1 - g\,. \tag{B.4b}$$

Therefore, eq. (B.3) becomes

$$\Phi_P = A_U\Phi_W + C_U\Phi_N + D_U\Phi_S\,, \tag{B.5a}$$

where

$$A_U = \frac{(A_C + fB_C)}{1 - gB_C}\,, \qquad C_U = \frac{C_C}{1 - gB_C}\,, \qquad D_U = \frac{D_C}{1 - gB_C}\,. \tag{B.5b}$$

These are the exact coefficients in eq. (29). The corresponding approximate coefficients in eq. (30) (corresponding to a scheme in which the UAC is used with an "exact" representation of diffusion) are obtained by setting $\alpha_e = \alpha_w = 1/2$ in the equations for A_C, C_C, D_C and substituting these new (approximate) values into eq. (B.5b). Upon this substitution, A_U, C_U and D_U become respectively, a_U, c_U and d_U.

Appendix C. Transient convection

(a) *Determination of coefficients*

The integral counterpart of eq. (18) for the volume surrounding P in fig. 1 over the time interval

Δt is

$$-\frac{1}{\Delta x}\int\limits_{x_w}^{x_e}(\Phi^{t+\Delta t}-\Phi^t)\,dx=\left[\frac{u\Delta t}{\Delta x}\right]\left\{\frac{1}{\Delta t}\int\limits_{t}^{t+\Delta y}[(\Phi)_e-(\Phi)_w]\,dt\right\}. \tag{C.1}$$

The left-hand side, with the knowledge of the exact solution in eq. (34), can be replaced without approximation by

$$[\Phi_P^{t+\Delta t}-\Phi_P^t]\,\frac{\sin(\tilde{x}/2)}{(\tilde{x}/2)},$$

where $\tilde{x}=\omega\Delta x/u$, and where the grid spacing is uniform in the x direction. According to the UAC, the other term would be *approximated* by $[\Phi_P-\Phi_W]^{t+\kappa\Delta t}$, where $t+\kappa\Delta t$ is the reference time such that

$$\Phi_P^{t+\kappa\Delta t}=(1-\kappa)\Phi_P^t+\kappa\Phi_P^{t+\Delta t} \tag{C.2}$$

Substituting this approximation into the right-hand side of (C.1), replacing the left-hand side by the "exact" expression above and replacing Φ by ϕ in recognition that the resulting equation is only an approximation to the exact equation for Φ, results in eq. (35), wherein

$$a_\kappa=\frac{1-c^*(1-\kappa)}{1+c^*\kappa},\qquad b_\kappa=\frac{c^*(1-\kappa)}{1+c^*\kappa},\qquad d_\kappa=\frac{c^*\kappa}{1+c^*\kappa}, \tag{C.3a}$$

where

$$c^*=\frac{u\Delta t}{\Delta x}\,\frac{\tilde{x}/2}{\sin(\tilde{x}/2)} \tag{C.3b}$$

is a modified Courant number, and $t=n\Delta t$.

The corresponding values of A_κ, B_κ and D_κ in eq. (36) can be found by susbtituting eq. (34) into (36). To determine unique values, one more constraint can be applied. Here, $b_\kappa/d_\kappa=B_\kappa/D_\kappa$ was used. The result, using the notation $\tilde{x}=\omega\Delta x/u$ and $\tilde{t}=\omega\Delta t$, is

$$A_\kappa=[(1-\kappa)\sin(\tilde{x}-\tilde{t})+\kappa\sin(\tilde{x})]/F,\qquad B_\kappa=(1-\kappa)\sin(\tilde{t})/F,\qquad D_\kappa=\kappa\sin(\tilde{t})/F, \tag{C.4}$$

where $F=(1-\kappa)\sin\tilde{x}+\kappa\sin(\tilde{x}+\tilde{t})$.

It can be seen that as $\tilde{x}\to 0$ and $\tilde{t}\to 0$, it follows that $a_\kappa\to A_\kappa$ etc.

(b) *Error analysis*

Eq. (37) constitutes an approximate upper bound on the error in ϕ arising from the use of an UAC. With the understanding that the subscript κ is dropped for ease in writing, the coefficient errors are

$$\delta a=a-A,\qquad \delta b=b-B,\qquad \delta d=d-D. \tag{C.5}$$

Eqs. (35) and (36) subtract to give

$$e_{\mathrm{P}}^{n+1} = A e_{\mathrm{P}}^{n} + B e_{\mathrm{W}}^{n} + D e_{\mathrm{W}}^{n+1} + \delta a \phi_{\mathrm{P}}^{n} + \delta b \phi_{\mathrm{W}}^{n} + \delta d \, \phi_{\mathrm{W}}^{n+1} \, , \tag{C.6}$$

where $e_{\mathrm{P}}^{n} = \phi_{\mathrm{P}}^{n} - \Phi_{\mathrm{P}}^{n}$ etc.

Eq. (C.6) applies to each grid point but will not have the same value of e_{P}^{n+1} at each grid point. Letting E^{n+1} be the maximum value of e_{P}^{n+1} for any grid point at the $(n+1)$th time-level, we find

$$(1 - |D|)E^{n+1} \leqslant (|A| + |B|)E^{n} + (|\delta a| + |\delta b|)\,|\phi^{n}|_{\mathrm{MAX}} + |\delta d|\,|\phi^{n+1}|_{\mathrm{MAX}} \, , \tag{C.7}$$

where $|\phi^{n}|_{\mathrm{MAX}}$ is the maximum magnitude of ϕ at the nth time level. From eq. (35)

$$|\phi^{n+1}|_{\mathrm{MAX}} \leqslant \frac{|a^{\kappa}| + |b^{\kappa}|}{1 - |d^{\kappa}|}\,|\phi^{n}|_{\mathrm{MAX}} \, . \tag{C.8}$$

Combining (C.7) and (C.8), one obtains a recursion relation for E^{n+1} in terms of E^{n}. Performing a sum and using $E^{0} = 0$ (that is the initial conditions are without error) results in

$$E^{n+1} \leqslant \beta^{*} \left\{ \frac{1 - \alpha^{n+1}}{1 - \alpha} \right\} \, , \tag{C.9}$$

where

$$\beta^{*} = \left\{ |\delta a| + |\delta b| + |\delta d| \left(\frac{|a| + |b|}{1 - |d|} \right) \right\} \left\{ \frac{|a| + |b|}{1 - |d|} \right\}^{n-1} \quad \{1 - |D|\}$$

and

$$\alpha = (|A| + |B|)/(1 - |D|) \, .$$

Eq. (C.9) is an upper bound on the error growth. When all the coefficients a, b and d are positive, then

$$|a| + |b| + |d| = 1 \qquad \text{and} \qquad |A| + |B| + |D| = 1 + \epsilon \, ,$$

where ϵ is a small number, so that (C.9) simplifies to eq. (37).

The above error is attributed to the UAC alone. If c^{*} in eq. (C.3b) were replaced by $c = u\Delta t/\Delta x$, the error above would become the error due to approximating *both* the transient and convection term.

(c) *Modified Leith analysis*

A better method of approximating the right hand side of eq. (C.1) is

$$\frac{1}{\Delta t} \int_{t}^{t+\Delta t} (\Phi_{\mathrm{e}} - \Phi_{\mathrm{w}})\,\mathrm{d}t \approx \Phi(x_{\mathrm{e}}, t + \Delta t/2) - \Phi(x_{\mathrm{w}}, t + \Delta t/2) \, . \tag{C.10}$$

However, for the problem at hand, $\Phi(x_e, t + \Delta t/2) = \Phi(x_e - u\Delta t/2, t)$, which, using a linear interpolation in space, becomes

$$\Phi(x_e - u\Delta t/2, t) \approx \Phi_E^t + \{\tfrac{1}{2} + \tfrac{1}{2}c\}(\Phi_P^t - \Phi_E^t)\,, \tag{C.11}$$

where $c = u\Delta t/\Delta x$ is the Courant number. Substituting these approximations into (C.1), where the left-hand side is replaced by the "exact" formulation, and where ϕ replaces Φ as a reminder that the equation is approximate, one obtains

$$\phi_P^{t+\Delta t} = [1 - c^* c]\phi_P^t + \tfrac{1}{2}c^*(c-1)\phi_E^t + \tfrac{1}{2}c^*(c+1)\phi_W^t\,. \tag{C.12}$$

The error in $\phi_P^{t+\Delta t}$ arising from the use of eq. (C.12) is attributed to the error in approximating the convection terms in the sense that *if* the convection terms had been approximated exactly, then the conservation equation would be exactly satisfied.

If one wishes to include also the error in the transient term approximation, c^* is replaced by c and Leith's scheme [16] results.

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