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A STUDY OF UPSTREAM-WEIGHTED HIGH-ORDER DIFFERENCING FOR APPROXIMATION TO FLOW CONVECTION

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SUMMARY

This paper is concerned with a number of upstream-weighted second- and third-order difference schemes. Also considered are the conventional upwind and central difference schemes for comparison. It commences with a general difference equation which unifies all the given first-, second- and third-order schemes. The various schemes are evaluated through the use of the general equation. The unboundedness and accuracy of the solutions by the difference schemes are assessed via various analyses: examination of the coefficients of the difference equation, Taylor series truncation error analysis, study of the upstream connection to numerical diffusion, single-cell analysis. Finally, the difference schemes are tested on one- and two-dimensional model problems. It is shown that the high-order schemes suffer less from the problem of numerical diffusion than the first-order upwind difference scheme. However, unboundedness cannot be avoided in the solutions by these schemes. Among them the linear upwind difference scheme presents the best compromise between numerical diffusion and solution unboundedness.

KEY WORDS Finite difference High-order schemes Numerical diffusion Solution unboundedness

1. INTRODUCTION

In a lot of fluid flow problems the flow velocity in part of the domain of interest is so high that the flow transport is dominated by convection. In the numerical simulation of fluid flow, such as the finite difference method, the difference approximation to the terms in the governing equations representing convection is so important that not only does the accuracy of the final solutions depend on the choice of approximation but the stability of the solution procedure is also affected.

Traditionally the second-order-accurate central difference (CD) and first-order-accurate upwind difference (UD) are used to simulate the first-order derivatives of the convection terms.[1] The basis of the central difference is that the face value transported across a cell surface is approximated by linear weighting between the nearest two nodal points (Figure 1(a)). The major problem encountered by the central difference scheme is that unphysical oscillations may appear in the solution as the Reynolds (or Peclet) number becomes sufficiently large and thus the solution may diverge unless special treatments are undertaken.[2] The remedy has been to use the upwind difference in regions where the convection becomes dominant.[3,4] For the upwind difference a zero-order extrapolation from the upstream point is made to give the convected face value

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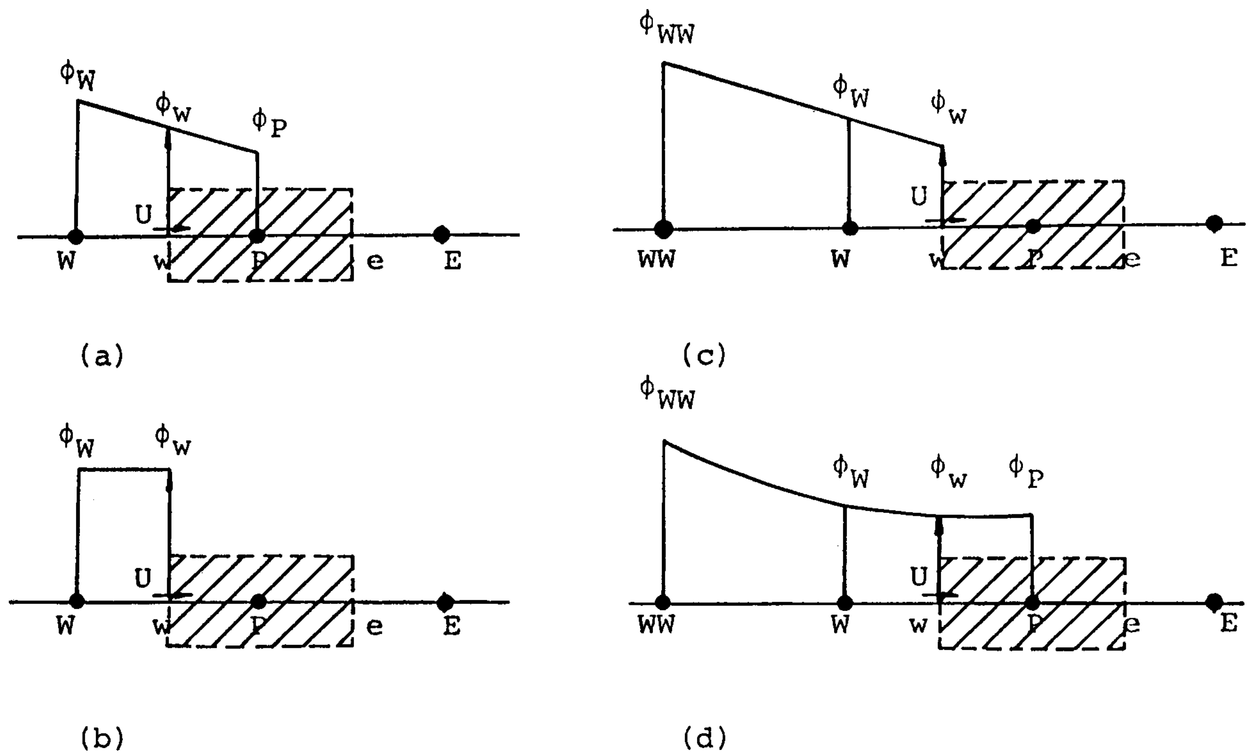


Figure 1. Illustration of spatial differencings: (a) central difference; (b) upwind difference; (c) linear upwind difference; (d) quadratic upwind difference

(Figure 1(b)). By using the upwind difference, all the coefficients linking the principal node to the neighbouring nodes are of the same sign. As a result, the coefficient matrix is diagonally dominant and no solution oscillations occur. Taylor series analysis indicates that the leading truncated term of the upwind difference is of second-order differential form with the coefficient linearly proportional to the grid size. Thus the upwind difference inherently has the nature of dissipation. It can be seen that the upwind difference is equivalent to the 'non-dissipative' second-order-accurate central difference with added dissipation. The dissipative nature helps to smooth out disturbances and stabilize the solution. However, the stability is achieved at the expense of accuracy: the numerical dissipation may obscure the physical processes. For example, in the case of high Reynolds number the eddy viscosity may be overshadowed by the artificial viscosity of the numerical diffusion. This problem becomes more serious when the streamlines are not aligned with the grid co-ordinates.[5] Because of this, numerical procedures using the hybrid upwind/central difference for turbulent recirculating flows have been found to underpredict the dimensions of the recirculation region.[6,7] The effect of numerical diffusion can be alleviated by the exercise of grid refinement. However, the cost sometimes is too high, especially when a complicated geometry is involved and/or the flow is three-dimensional. A more promising approach is to adopt an upstream-weighted higher-order difference instead of the upwind difference.

In the past few years several high-order difference schemes have emerged and have been used in predictions of the full Navier–Stokes equations. Two of them are second-order-accurate: the quadratic upwind difference (QUD) (or the QUICK scheme, as named by Leonard[8]) and the linear upwind difference (LUD).[9,10] The two schemes proposed by Agarwal[11] and Kawamura and Kuwahara[12] are one order higher, i.e. third-order-accurate.

In the linear upwind difference the face value is yielded via a two-point extrapolation with the two points in question located in the upstream direction (Figure 1(c)), while the quadratic upwind difference is based upon a three-point quadratic interpolation with two points upstream and one point downstream of the cell face (Figure 1(d)). These two schemes have been tested and evaluated by a number of research workers.[6–10,13–22] In general, the two schemes give better results than the hybrid upwind/central difference using the same grids. However, although much less serious than with the central difference, overshoots and/or undershoots may appear in the solutions because the coefficient matrices are not diagonally dominant. The oscillations are obvious when the schemes are applied to simple one-dimensional and two-dimensional model equations which mimic the Navier–Stokes equations for high-Reynolds-number flow. Another major drawback of these high-order schemes is that they require more iterations and thus more computer time to converge than the hybrid scheme, since iterative methods such as the point and line relaxation methods and Stone's strongly implicit procedure[23] are used. The other two schemes, which are more 'accurate' than the QUD and LUD in terms of truncation error, have not attracted much attention and their characteristics have not been fully unveiled yet, though they have been successfully applied to recirculating flow calculations by their inventors.[11,12] Therefore they deserve further exploration.

In this study a general difference scheme is devised. From this scheme the above-mentioned schemes can easily be deduced by assigning appropriate values to the relevant parameters. In addition, new difference schemes can also be derived. A total of eight difference schemes are considered. Another advantage of using the general scheme is that it is not necessary to repeat the same practice in the analysis for each of the schemes. The study includes examination of the coefficients of the difference equation, Taylor series analysis, upwind connection to numerical diffusion, single-cell analysis and one- and two-dimensional model problem studies.

2. GENERAL DIFFERENCE FORM

Consider the convection of a general scalar entity ϕ in the x-direction, $u\partial\phi/\partial x$, where u is the flow velocity. The spatial derivative may be approximated in the following manner:

$$\frac{\partial\phi}{\partial x}=\frac{1}{\Delta x}(\phi_e-\phi_w), \tag{1}$$

where ϕ_e and ϕ_w are the face values at the east and west surfaces of the considered cell respectively. Different schemes are obtained through different approximations to the face values, obtained by linear weighting of the neighbouring nodal values. As discussed in the above and shown in Figure 1, the face values of the UD, CD, LUD and QUD schemes are evaluated by zero-order extrapolation, linear interpolation, linear extrapolation and quadratic interpolation respectively. By assuming the velocity u to be positive, these schemes can be expressed as follows:

upwind difference (UD)

$$\phi_e=\phi_P, \tag{2a}$$

$$\phi_w=\phi_W; \tag{2b}$$

central difference (CD)

$$\phi_e=\tfrac{1}{2}(\phi_E+\phi_P), \tag{3a}$$

$$\phi_w=\tfrac{1}{2}(\phi_P+\phi_W); \tag{3b}$$

linear upwind difference (LUD)

$$\phi_e=\tfrac{3}{2}\phi_P-\tfrac{1}{2}\phi_W, \tag{4a}$$

$$\phi_w=\tfrac{3}{2}\phi_W-\tfrac{1}{2}\phi_{WW}; \tag{4b}$$

quadratic upwind difference (QUD, i.e. the QUICK scheme of Leonard[8])

$$\phi_e=\tfrac{3}{8}\phi_E+\tfrac{3}{4}\phi_P-\tfrac{1}{8}\phi_W, \tag{5a}$$

$$\phi_w=\tfrac{3}{8}\phi_P+\tfrac{3}{4}\phi_W-\tfrac{1}{8}\phi_{WW}. \tag{5b}$$

The upwind difference can be arranged to give

$$\frac{\partial\phi}{\partial x}=\frac{1}{\Delta x}(\phi_P-\phi_W)=\frac{1}{\Delta x}[\tfrac{1}{2}(\phi_E-\phi_W)-\tfrac{1}{2}(\phi_E-2\phi_P+\phi_W)]. \tag{6}$$

The second term in brackets is an approximation to $(\Delta x/2)\partial^2\phi/\partial x^2$, implying that the upwind difference is equivalent to a central difference with artificial dissipation. The coefficient $\Delta x/2$ represents the viscosity of the artificial dissipation. If the multiplier $\frac{1}{2}$ is replaced by an arbitrary value α, we have

$$\frac{\partial\phi}{\partial x}=\frac{1}{\Delta x}[\tfrac{1}{2}(\phi_E-\phi_W)-\alpha(\phi_E-2\phi_P+\phi_W)]. \tag{7}$$

This is a general first-order difference scheme because its truncation error is $\alpha\Delta x\partial^2\phi/\partial x^2$. Obviously α must be greater than zero to give positive artificial viscosity. By this scheme the transported values at the cell surfaces are evaluated as

$$\phi_e = \tfrac{1}{2}(\phi_E + \phi_P) - \alpha(\phi_E - \phi_P), \tag{8a}$$

$$\phi_w = \tfrac{1}{2}(\phi_P + \phi_W) - \alpha(\phi_P - \phi_W). \tag{8b}$$

The above expressions can be recast into the following form, e.g.

$$\phi_w = f\phi_P + (1-f)\phi_W, \tag{9}$$

where $f = \frac{1}{2} - \alpha$. It is clear that for $0 < f < 1$ (i.e. $-\frac{1}{2} < \alpha < \frac{1}{2}$) a linear interpolation between ϕ_P and ϕ_W is employed to yield ϕ_w (Figure 2(b)). For $f < 0$ (i.e. $\alpha > \frac{1}{2}$) a value obtained through linear extrapolation from ϕ_P and ϕ_W to a point w′ upstream of the point W is implied (Figure 2(a)). The case $f > 1$ (i.e. $\alpha < -\frac{1}{2}$), which is the most unfavoured, implies that ϕ_w is obtained by linear extrapolation to a point downstream of the point P (Figure 2(c)).

The CD, LUD and QUD can be cast into the following form:

$$\frac{\partial \phi}{\partial x} = \frac{1}{\Delta x}\left[\tfrac{1}{2}(\phi_E - \phi_W) - \alpha(\phi_E - 2\phi_P + \phi_W) + \alpha(\phi_P - 2\phi_W + \phi_{WW})\right], \tag{10}$$

which is equivalent to setting

$$\phi_e = \tfrac{1}{2}(\phi_E + \phi_P) - \alpha(\phi_E - 2\phi_P + \phi_W), \tag{11a}$$

$$\phi_w = \tfrac{1}{2}(\phi_P + \phi_W) - \alpha(\phi_P - 2\phi_W + \phi_{WW}), \tag{11b}$$

where

$$\alpha = \begin{cases} 0 & \text{for the CD,} \\ \frac{1}{2} & \text{for the LUD,} \\ \frac{1}{8} & \text{for the QUD.} \end{cases}$$

Since the artificial dissipations represented by the second and third terms on the right-hand side of equation (10) cancel each other, it is at least second-order-accurate irrespective of the value of α. The leading truncated term of the difference approximation is $(\frac{1}{6} - \alpha)\Delta x^2 \partial^3\phi/\partial x^3$. It is obvious that this term disappears when $\alpha = \frac{1}{6}$, which is the scheme proposed by Agarwal.[11] In order to

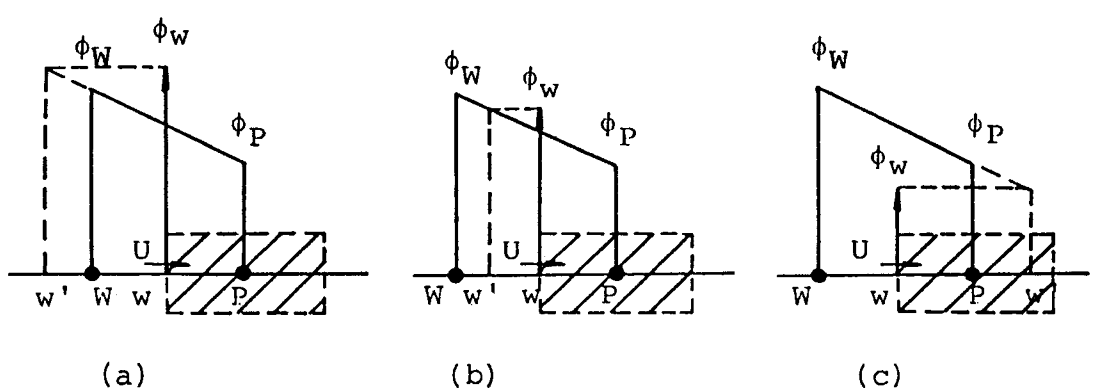


Figure 2. Schematic illustration of interpolation/extrapolation practices implied by α for the general first-order scheme: (a) $\alpha > \frac{1}{2}$; (b) $-\frac{1}{2} < \alpha < \frac{1}{2}$; (c) $\alpha < -\frac{1}{2}$

enhance the order of accuracy when α not equal to $\frac{1}{6}$, the third-order derivative of the leading truncated term can be discretized as

$$\frac{\partial^3\phi}{\partial x^3}=\frac{1}{2\Delta x}[(\phi_{EE}-2\phi_E+\phi_P)-(\phi_P-2\phi_W+\phi_{WW})]. \tag{12}$$

Thus a third-order scheme can be obtained:

$$\begin{aligned}\frac{\partial\phi}{\partial x}=\frac{1}{\Delta x}[&\tfrac{1}{2}(\phi_E-\phi_W)-\alpha(\phi_E-2\phi_P+\phi_W)+\alpha(\phi_P-2\phi_W+\phi_{WW})\\&+\tfrac{1}{2}(\alpha-\tfrac{1}{6})(\phi_{EE}-2\phi_E+\phi_P)-\tfrac{1}{2}(\alpha-\tfrac{1}{6})(\phi_P-2\phi_W+\phi_{WW})].\end{aligned} \tag{13}$$

By choosing $\alpha=\frac{1}{2}$ we have the scheme proposed by Kawamura and Kuwahara.[12]

The first-, second- and third-order schemes can be unified to give

$$\begin{aligned}\frac{\partial\phi}{\partial x}&=\frac{1}{\Delta x}[\tfrac{1}{2}(\phi_E-\phi_W)-\alpha(\phi_E-2\phi_P+\phi_W)+\beta(\phi_P-2\phi_W+\phi_{WW})\\&\quad+\tfrac{1}{2}\gamma(\phi_{EE}-2\phi_E+\phi_P)-\tfrac{1}{2}\gamma(\phi_P-2\phi_W+\phi_{WW})]\\&=\frac{1}{\Delta x}[\tfrac{1}{2}\gamma\phi_{EE}+(\tfrac{1}{2}-\alpha-\gamma)\phi_E+(2\gamma+\beta)\phi_P+(-\tfrac{1}{2}-\alpha-2\beta+\gamma)\phi_W+(\beta-\tfrac{1}{2}\gamma)\phi_{WW}],\end{aligned} \tag{14}$$

where

$$\begin{cases}\beta=0,\ \gamma=0\text{: first-order scheme, equation (7),}\\ \alpha=\beta,\ \gamma=0\text{: second-order scheme, equation (10),}\\ \alpha=\beta,\ \gamma=\alpha-\tfrac{1}{6}\text{: third-order scheme, equation (13).}\end{cases}$$

The face values are evaluated

$$\phi_e=\tfrac{1}{2}(\phi_E+\phi_P)-\alpha(\phi_E-\phi_P)+\beta(\phi_P-\phi_W)+\tfrac{1}{2}\gamma(\phi_{EE}-\phi_E)-\tfrac{1}{2}\gamma(\phi_P-\phi_W), \tag{15a}$$

$$\phi_w=\tfrac{1}{2}(\phi_P+\phi_W)-\alpha(\phi_P-\phi_W)+\beta(\phi_W-\phi_{WW})+\tfrac{1}{2}\gamma(\phi_E-\phi_P)-\tfrac{1}{2}\gamma(\phi_W-\phi_{WW}). \tag{15b}$$

The expressions for ϕ_e and ϕ_w are of the same form except that the nodal points involved are shifted by one grid size. Therefore the conservative property of the differential equation is preserved. It needs to be noted that the second-order central difference is a special case of the general first-order difference scheme: $\alpha=\beta=\gamma=0$; and the third-order Agarwal scheme is a special case of the general second-order scheme: $\alpha=\beta=\frac{1}{6}$ and $\gamma=0$. A summary of the assignment of the parameters for the different schemes is given in Table I. In the table the Agarwal scheme is denoted

Table I. Assignments of parameters for various schemes.

	$\gamma=0$		$\gamma=\alpha-\frac{1}{6}$
	$\beta=0$ (first-order scheme)	$\beta=\alpha$ (second-order scheme)	$\beta=\alpha$ (third-order scheme)
$\alpha=0$	CD	CD	—
$\alpha=\frac{1}{2}$	UD	LUD	ELUD
$\alpha=\frac{1}{3}$	—	—	CUD($\frac{1}{3}$)
$\alpha=\frac{1}{6}$	—	CUD($\frac{1}{6}$)	CUD($\frac{1}{6}$)
$\alpha=\frac{1}{8}$	—	QUD	EQUD

as CUD($\frac{1}{6}$) (cubic upwind difference) and the Kawamura–Kuwahara scheme as ELUD (extended LUD). Two additional third-order schemes, which correspond to $\alpha=\frac{1}{3}$ and $\frac{1}{8}$ respectively and will be discussed later, are also shown and denoted as CUD($\frac{1}{3}$) and EQUD (extended QUD).

3. EXAMINATION OF THE COEFFICIENTS

Consider a one-dimensional transport equation:

$$u\frac{\mathrm{d}\phi}{\mathrm{d}x}=\Gamma\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}, \tag{16}$$

where Γ is the diffusivity. By using the standard central difference approximation for the diffusion and equation (14) for the convection, the difference analogue of the above equation is given by

$$A_\mathrm{P}\phi_\mathrm{P}=A_\mathrm{E}\phi_\mathrm{E}+A_\mathrm{W}\phi_\mathrm{W}+A_\mathrm{EE}\phi_\mathrm{EE}+A_\mathrm{WW}\phi_\mathrm{WW}. \tag{17}$$

The coefficients are defined as

$$A_\mathrm{E}=(-\tfrac{1}{2}+\alpha+\gamma)+1/Pe, \tag{18a}$$

$$A_\mathrm{W}=(\tfrac{1}{2}+\alpha+2\beta-\gamma)+1/Pe, \tag{18b}$$

$$A_\mathrm{EE}=-\tfrac{1}{2}\gamma, \tag{18c}$$

$$A_\mathrm{WW}=-\beta+\tfrac{1}{2}\gamma, \tag{18d}$$

$$A_\mathrm{P}=2\alpha+\beta+2/Pe=\sum A_c,\quad c=\mathrm{E, W, EE, WW}, \tag{18e}$$

where $Pe=u\Delta x/\Gamma$ is the cell Peclet number. The coefficients for each difference scheme are listed in Table II. In Table III the coefficients are divided by the central coefficient for infinite Peclet number. For the pure transport problem the values of transported quantities in the interior of the flow field should be within the range bounded by boundary values. To ensure diagonal dominance of the coefficient matrix as well as 'boundedness' of the solution, all the coefficients of equation (18) should be of the same sign. Violation of this regulation may cause unboundedness in the solution, i.e. solution oscillations. Besides, when a relaxation method is used to solve the system of discrete equations, it may result in numerical instability, since the coefficient matrix is not diagonally dominant, unless underrelaxation is taken. To indicate to what extent the difference schemes deviate from diagonal dominance and boundedness, the last column of Table III gives the ratio of the absolute sum of the neighbouring coefficients to the central coefficient. Some interesting points can be drawn from the tables.

First we examine the first-order scheme. It is obvious from Table III that the weighted coefficient $A_\mathrm{E}/A_\mathrm{P}$ is non-negative and $\sum|A_c|/A_\mathrm{P}$ is equal to one when $\alpha\geq\frac{1}{2}$. Hence upstream extrapolations ($\alpha\geq\frac{1}{2}$, see Figure 2(a)) do not impair diagonal dominance. Since the truncation error is linearly proportional to α, the zero extrapolation of the standard upwind difference ($\alpha=\frac{1}{2}$) is the most accurate among the extrapolations.

It is seen from Table II that the east coefficient A_E of the central difference becomes negative when the cell Peclet number becomes larger than two. It is unconditionally unbounded as Pe approaches infinity because the central coefficient A_P is zero and thus the neighbouring weighted coefficients $A_\mathrm{W}/A_\mathrm{P}$ and $A_\mathrm{E}/A_\mathrm{P}$ become positive and negative infinities respectively. For the other second-order schemes Table III reveals that a constant negative coefficient $A_\mathrm{WW}/A_\mathrm{P}$ ($=-\frac{1}{3}$) emerges, ruling out any possibility for these schemes to avoid unboundedness. Furthermore, the principal coefficient $A_\mathrm{E}/A_\mathrm{P}$ ($=\frac{1}{3}-\frac{1}{6}\alpha$) becomes negative for $0<\alpha<\frac{1}{2}$. From Table II it can be seen that A_E is negative when $Pe>3$ for the CUD($\frac{1}{6}$) ($\alpha=\frac{1}{6}$) and $Pe>\frac{8}{3}$ for the QUD ($\alpha=\frac{1}{8}$). As for $\alpha\geq\frac{1}{2}$,

Table II. Coefficients for various schemes in one-dimensional steady flow

Scheme	Coefficient				
	A_{WW}	A_W	A_E	A_{EE}	A_P
General form	$-(\beta-\frac{1}{2}\gamma)$	$(\frac{1}{2}+\alpha+2\beta-\gamma)+1/Pe$	$(-\frac{1}{2}+\alpha+\gamma)+1/Pe$	$-\frac{1}{2}\gamma$	$(2\alpha+\beta)+2/Pe$
First-order ($\beta=\gamma=0$)	0	$(\alpha+\frac{1}{2})+1/Pe$	$(\alpha-\frac{1}{2})+1/Pe$	0	$2\alpha+2/Pe$
UD ($\alpha=\frac{1}{2}$)	0	$1+1/Pe$	$1/Pe$	0	$1+2/Pe$
Second-order ($\alpha=\beta$, $\gamma=0$)	$-\alpha$	$(3\alpha+\frac{1}{2})+1/Pe$	$(\alpha-\frac{1}{2})+1/Pe$	0	$3\alpha+2/Pe$
CD ($\alpha=\beta=0$)	0	$\frac{1}{2}+1/Pe$	$-\frac{1}{2}+1/Pe$	0	$2/Pe$
LUD ($\alpha=\beta=\frac{1}{2}$)	$-\frac{1}{2}$	$2+1/Pe$	$1/Pe$	0	$\frac{3}{2}+2/Pe$
QUD ($\alpha=\beta=\frac{1}{6}$)	$-\frac{1}{8}$	$\frac{7}{8}+1/Pe$	$-\frac{3}{8}+1/Pe$	0	$\frac{3}{8}+2/Pe$
Third-order ($\alpha=\beta$, $\gamma=\alpha-\frac{1}{6}$)	$-(\frac{1}{12}+\frac{1}{2}\alpha)$	$(\frac{2}{3}+2\alpha)+1/Pe$	$(-\frac{2}{3}+2\alpha)+1/Pe$	$\frac{1}{12}-\frac{1}{2}\alpha$	$3\alpha+2/Pe$
ELUD ($\alpha=\beta=\frac{1}{2}$)	$-\frac{1}{3}$	$\frac{5}{3}+1/Pe$	$\frac{1}{3}+1/Pe$	$-\frac{1}{6}$	$\frac{3}{2}+2/Pe$
CUD($\frac{1}{3}$) ($\alpha=\beta=\frac{1}{3}$)	$-\frac{1}{4}$	$\frac{4}{3}+1/Pe$	$1/Pe$	$-\frac{1}{12}$	$1+2/Pe$
CUD(1/6) ($\alpha=\beta=\frac{1}{6}$)	$-\frac{1}{6}$	$1+1/Pe$	$-\frac{1}{3}+1/Pe$	0	$\frac{1}{2}+2/Pe$
EQUD ($\alpha=\beta=\frac{1}{8}$)	$-\frac{7}{48}$	$\frac{11}{12}+1/Pe$	$-\frac{5}{12}+1/Pe$	$\frac{1}{48}$	$\frac{3}{8}+2/Pe$

the LUD scheme ($\alpha=\frac{1}{2}$) is the most accurate according to the Taylor series truncation error analysis. Comparing $\sum|A_c|/A_P$ suggests that the unboundedness of the LUD solution is the least serious. The QUD is most likely to suffer from this problem, seriously undermining stability. The CUD($\frac{1}{6}$) is in between.

For the third-order schemes the weighted coefficient A_{WW}/A_P is negative, but no longer constant as for the second-order schemes. It varies from $-\frac{2}{9}$ for the ELUD to $-\frac{7}{18}$ for the EQUD. The third-order schemes, not including CUD($\frac{1}{6}$), require four points, two upstream and two downstream, to evaluate the convected face values, while for the second-order schemes not more than three points, two upstream and one downstream, are involved. Hence the far east downstream coefficients A_{EE}/A_P of the third-order schemes are non-zero: $-\frac{1}{9}$ for the ELUD, $-\frac{1}{12}$ for the CUD($\frac{1}{3}$) and $\frac{1}{18}$ for the EQUD. As for the coefficient A_E, it becomes negative for the EQUD when Pe is larger than $\frac{12}{5}$. For infinite Pe the weighted coefficient A_E/A_P is $\frac{2}{9}$, 0 and $-\frac{10}{9}$ for the ELUD, CUD($\frac{1}{3}$) and EQUD respectively. It is interesting to note that the sum of the far neighbouring coefficients $A_{WW}/A_P+A_{EE}/A_P$ is the same for each third-order scheme and its corresponding second-order scheme, and so is the sum of the principal coefficients $A_W/A_P+A_E/A_P$.

The absolute sum $|A_c|/A_P$ is plotted against α for all the schemes in Figure 3. The three curves represent the three general difference schemes. When α is close to zero, the values of the sum for all the schemes approach infinity, implying that the solutions of all the schemes would be unbounded.

Table III. Weighted coefficients for various schemes in one-dimensional steady flow at infinite Peclet number

Scheme	Coefficient				
	A_{WW}/A_P	A_W/A_P	A_E/A_P	A_{EE}/A_P	$\sum \lvert A_c\rvert/A_P$
CD ($\alpha=\beta=0$)	0	∞	$-\infty$	0	∞
General form	$\frac{-(\beta-\frac{1}{2}\gamma)}{2\alpha+\beta}$	$\frac{\frac{1}{2}+\alpha+2\beta-\gamma}{2\alpha+\beta}$	$\frac{\frac{1}{2}+\alpha+\gamma}{2\alpha+\beta}$	$\frac{-\gamma}{4\alpha+2\beta}$	—
First-order ($\beta=\gamma=0$)	0	$\frac{1}{2}+1/4\alpha$	$\frac{1}{2}-1/4\alpha$	0	$1/2\alpha$ (i), 1 (ii)
UD ($\alpha=0$)	0	1	0	0	1
Second-order ($\alpha=\beta$, $\gamma=0$)	$-\frac{1}{3}$	$1+1/6\alpha$	$\frac{1}{3}-1/6\alpha$	0	$1+1/3\alpha$ (i), $\frac{5}{3}$ (ii)
LUD ($\alpha=\beta=\frac{1}{2}$)	$-\frac{1}{3}$	$\frac{4}{3}$	0	0	$\frac{5}{3}$
QUD ($\alpha=\beta=\frac{1}{6}$)	$-\frac{1}{3}$	$\frac{7}{3}$	-1	0	$\frac{11}{3}$
Third-order ($\alpha=\beta$, $\gamma=\alpha-\frac{1}{6}$)	$-(\frac{1}{6}+1/36\alpha)$	$\frac{2}{3}+2/9\alpha$	$\frac{2}{3}-2/9\alpha$	$-\frac{1}{6}+1/36\alpha$	$\frac{5}{3}$ (iii), $\frac{1}{3}+4/9\alpha$ (iv), $\frac{1}{2\alpha}$ (v)
ELUD ($\alpha=\beta=\frac{1}{2}$)	$-\frac{2}{9}$	$\frac{10}{9}$	$\frac{2}{9}$	$-\frac{1}{9}$	$\frac{5}{3}$
CID($\frac{1}{3}$) ($\alpha=\beta=\frac{1}{3}$)	$-\frac{1}{4}$	$\frac{4}{3}$	0	$-\frac{1}{12}$	$\frac{5}{3}$
CUD($\frac{1}{6}$) ($\alpha=\beta=\frac{1}{6}$)	$-\frac{1}{3}$	2	$-\frac{2}{3}$	0	3
EQUD ($\alpha=\beta=\frac{1}{8}$)	$-\frac{7}{18}$	$\frac{22}{9}$	$-\frac{10}{9}$	$\frac{1}{18}$	4

(i) For $0<\alpha\leq\frac{1}{2}$.
(ii) For $\alpha\geq\frac{1}{2}$.
(iii) For $\alpha\geq\frac{1}{3}$.
(iv) For $\frac{1}{6}\leq\alpha\leq\frac{1}{3}$.
(v) For $0<\alpha\leq\frac{1}{6}$.

The two curves representing the first- and third-order schemes collapse into one for $\alpha\leq\frac{1}{16}$. They intersect with the other curve at $\alpha=\frac{1}{6}$. In the range $\frac{1}{6}<\alpha<\frac{1}{2}$ the curve for the third-order scheme lies between those for the other two schemes. It remains constant for $\alpha\geq\frac{1}{3}$ and intersects with the curve for the second-order scheme again at $\alpha=\frac{1}{2}$. On the basis of this observation it is argued that the LUD, ELUD and CUD($\frac{1}{3}$) may behave similarly. The sum of the first-order scheme is less than those for the high-order schemes for $\alpha\geq\frac{1}{6}$. It reaches and remains unity when α increases to $\frac{1}{2}$ and beyond.

4. TAYLOR SERIES ANALYSIS

Aside from round-off error the solution of a difference equation does not satisfy the original differential equation. The actual equation solved is called the modified equation[24] and is obtained by expanding each term of the difference equation into a Taylor series about the point where the

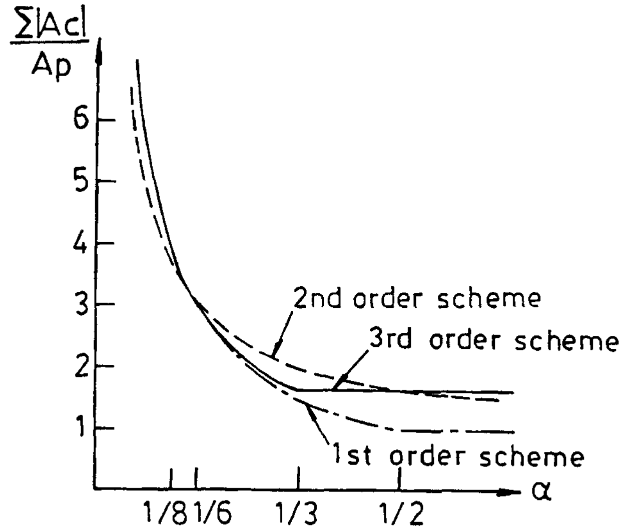


Figure 3. Variation of the ratio $\sum|A_c|/A_P$ with α for the first-, second- and third-order schemes

equation is located. Consider the case of purely convective transport

$$u\frac{d\phi}{dx}=0. \tag{19}$$

Its modified equation solved by the difference equation (14) is

$$u\frac{d\phi}{dx}=E_s, \tag{20}$$

where

$$E_s=\sum_{(n=2,4,\ldots)}\frac{-1}{n!}[(2^n-2)\beta-2\alpha]u(\Delta x)^{n-1}\frac{d^n\phi}{dx^n}$$
$$+\sum_{(n=3,5,\ldots)}\frac{-1}{n!}[(2^n-2)(\gamma-\beta)+1]u(\Delta x)^{n-1}\frac{d^n\phi}{dx^n}. \tag{21}$$

The term E_s is the truncation error introduced by the difference equation. To be clearer, the first few terms of E_s are given by

$$E_s\approx(\alpha-\beta)u(\Delta x)\frac{d^2\phi}{dx^2}+(\beta-\gamma-\tfrac{1}{6})u(\Delta x)^2\frac{d^3\phi}{dx^3}$$
$$+\tfrac{1}{12}(\alpha-7\beta)(\Delta x)^3\frac{d^4\phi}{dx^4}+[\tfrac{1}{4}(\beta-\gamma)-\tfrac{1}{120}](\Delta x)^4\frac{d^5\phi}{dx^5}. \tag{22}$$

As Δx becomes zero, the error vanishes and the modified equation is reduced to the original differential equation. Hence the finite difference equation is consistent with the given differential equation as Δx approaches zero.

The order of accuracy of a scheme is normally defined by the lowest-order power of the increment Δx of the truncation error. The even-order spatial derivatives have dissipative nature.[24] The first-order upwind scheme has a second-order derivative as its leading diffusion term with the coefficient linearly proportional to Δx. The lowest order of numerical diffusion for the second- and third-order schemes is a fourth-order derivative, of which the coefficient is proportional to the cube of Δx. Since the parameter γ does not appear in the even-number terms, any second-order scheme and its corresponding third-order scheme have the same numerical diffusion, and the central difference, for which $\alpha=\beta=0$, is non-dissipative.

In multidimensional flow the streamlines do not usually coincide with the grid lines. In the presence of skewness of the flow direction with respect to the grid co-ordinates, there exists cross-stream numerical diffusion in addition to the streamwise numerical diffusion discussed above. The cross-stream numerical diffusion of the upwind difference has been studied by a number of researchers.[13,25,26] In the following the approach used by Leschziner[13] is applied to the general difference scheme.

Consider a two-dimensional convective transport

$$u\frac{\partial\phi}{\partial x}+v\frac{\partial\phi}{\partial y}=0, \tag{23}$$

where u and v are the velocity components in the x- and y-directions. If the velocities u and v are assumed to be constant, the streamlines are straight lines at an angle $\theta=\tan^{-1}(v/u)$ to the x-axis. Using a transformation to transfer the above equation from the Cartesian co-ordinate system (x, y) to the streamline co-ordinate system (ξ, η), where ξ and η are the co-ordinates parallel and normal to the streamlines respectively, we obtain

$$V\frac{\partial\phi}{\partial\xi}=0, \tag{24}$$

where $V=u/\cos\theta=v/\sin\theta$ is the magnitude of the resultant velocity along the streamlines. It is obvious that ϕ is a constant along each streamline; however, it can be different on different streamlines. The modified equation can be derived by using the same transformation and ignoring all the derivatives involving $\partial/\partial\xi$ to the difference analogue of the above equation to obtain

$$V\frac{\partial\phi}{\partial\xi}=E_c, \tag{25}$$

where

$$\begin{aligned} E_c= & \sum_{(n=2,4,\ldots)}\frac{-1}{n!}[(2^n-2)\beta-2\alpha]\frac{V}{2}\sin(2\theta)(\cos^{n-1}\theta+\sin^{n-1}\theta)(\Delta x)^{n-1}\frac{\partial\phi^n}{\partial\eta^n} \\ & +\sum_{(n=3,5,\ldots)}\frac{-1}{n!}[(2^n-2)(\gamma-\beta)+1]\frac{V}{2}\sin(2\theta)(\cos^{n-1}\theta-\sin^{n-1}\theta)(\Delta x)^{n-1}\frac{\partial\phi^n}{\partial\eta^n}. \end{aligned} \tag{26}$$

The cross-stream error E_c depends on the normal derivatives $\partial^n\phi/\partial\eta^n$. It is also interesting to note that this error is a function of the flow angle θ. More about this error and the effect of the flow angle will be given in the later sections.

It should be pointed out that although the lowest-order power of Δx is referred to as the order of accuracy in the analysis, it cannot be truly representative of the error of the difference schemes. The effect of the high-order truncated terms may be as important as the lowest-order term and cannot be ignored. Evidence of this will be seen later.

5. THE UPWIND CONNECTION TO NUMERICAL DIFFUSION

It has been shown by the Taylor series analysis that all the difference schemes except the central difference inherently have dissipative character, which is of second order for the upwind difference and of fourth order for the others. Pulliam[27] has demonstrated that the UD scheme is equivalent to the non-dissipative CD scheme with a second-order artificial dissipation and that the LUD scheme is equivalent to a five-point central difference, not the standard three-point CD, with an added fourth-order dissipation. A similar concept can be generalized to the other upstream-weighted schemes given above as follows.

It is emphasized here that the difference scheme given by equation (14) is applicable only for positive velocity. For negative flow velocity u the corresponding difference is of the form

$$\frac{\partial\phi}{\partial x}=\frac{1}{\Delta x}[(-\beta+\tfrac{1}{2}\gamma)\phi_{EE}+(\tfrac{1}{2}+\alpha+2\beta-\gamma)\phi_E-(2\alpha+\beta)\phi_P+(-\tfrac{1}{2}+\alpha+\gamma)\phi_W-\tfrac{1}{2}\gamma\,\phi_{WW}]. \quad (27)$$

By denoting equation (14) as a backward differencing $\nabla\phi$ and equation (27) as a forward differencing $\Delta\phi$, a general form suitable for any flow direction is given:

$$u\frac{\partial\phi}{\partial x}=\frac{u}{2}(\nabla\phi+\Delta\phi)+\frac{|u|}{2}(\nabla\phi-\Delta\phi). \quad (28)$$

Obviously the right-hand side reduces to the backward differencing $u\nabla\phi$ for $u>0$ and the forward differencing $u\Delta\phi$ for $u<0$. The mean and half of the difference of the backward and forward differencings are given as

$$\tfrac{1}{2}(\nabla\phi+\Delta\phi)=-\tfrac{1}{2}(\beta-\gamma)\phi_{EE}+(\tfrac{1}{2}+\beta-\gamma)\phi_E-(\tfrac{1}{2}+\beta-\gamma)\phi_W+\tfrac{1}{2}(\beta-\gamma)\phi_{WW}, \quad (29a)$$

$$\tfrac{1}{2}(\nabla\phi-\Delta\phi)=\tfrac{1}{2}\beta\phi_{EE}-(\alpha+\beta)\phi_E+(2\alpha+\beta)\phi_P-(\alpha+\beta)\phi_W+\tfrac{1}{2}\beta\phi_{WW}. \quad (29b)$$

Expanding each term on the right-hand side of the above equations into Taylor series yields

$$\frac{u}{2}(\nabla\phi+\Delta\phi)=u\frac{\partial\phi}{\partial x}-E_{odd}, \quad (30a)$$

$$\frac{|u|}{2}(\nabla\phi-\Delta\phi)=-E_{even}, \quad (30b)$$

where

$$E_{odd}=\sum_{(n=3,5,\ldots)}\frac{-1}{n!}[(2^n-2)(\gamma-\beta)+1]u(\Delta x)^{n-1}\frac{\partial^n\phi}{\partial x^n}, \quad (31a)$$

$$E_{even}=\sum_{(n=2,4,\ldots)}\frac{-1}{n!}[(2^n-2)\beta-2\alpha]\,|u|\,(\Delta x)^{n-1}\frac{\partial^n\phi}{\partial x^n}. \quad (31b)$$

The error term E_{odd} is the same as the sum of the odd-number terms of E_s given by equation (21) and the other error term E_{even} is the same as the sum of the even-number terms of E_s. The mean $u(\nabla\phi+\Delta\phi)/2$ is a non-dissipative central difference scheme, which represents the standard CD scheme for the first-order upwind difference, a five-point second-order central difference for the second-order schemes and a five-point fourth-order central difference for the third-order schemes. The other term $|u|(\nabla\phi-\Delta\phi)/2$ is the added artificial dissipation, representing a second-order numerical diffusion for the first-order UD and a fourth-order diffusion for the high-order schemes. The dissipation term disappears when the standard CD is adopted. It is noted that (i) according to equation (29a) the embedded central differences for all the third-order schemes are identical since

$\beta-\gamma$ is a constant ($=\frac{1}{6}$) for these schemes and (ii) because equation (29b) is independent of γ, the dissipation is the same for any second-order scheme and its corresponding third-order scheme.

6. SINGLE-CELL ANALYSIS

As mentioned before, the high-order terms in the Taylor series analysis may not be small when compared with the low-order terms. This point will be clear in the analysis of this section. Here attention is confined to a single cell with mesh interval $\Delta x=0{\cdot}25$. The exact values are imposed on all the neighbouring nodal points apart from the central one. The solution at the central point, ϕ_P, by the chosen difference schemes is then evaluated. Such analysis is done on one-dimensional and two-dimensional cases. The CD scheme is excluded from this analysis.

6.1. One-dimensional analysis

The following one-dimensional equation is under consideration:

$$\frac{d\phi}{dx}=(m+1)x^m, \quad 0\leq x\leq 1. \tag{32}$$

The analytical solution of this equation is $\phi=x^{m+1}$. The errors between the numerical solutions and the analytical solution for the difference schemes are compared in Figure 4.

It is noted that $d^n\phi/dx^n=0$ for $n\geq m+1$ if m is an integer. If the solution ϕ is a quadratic function ($m=1$), all the high-order schemes give the exact solution as shown in Figure 4 since all

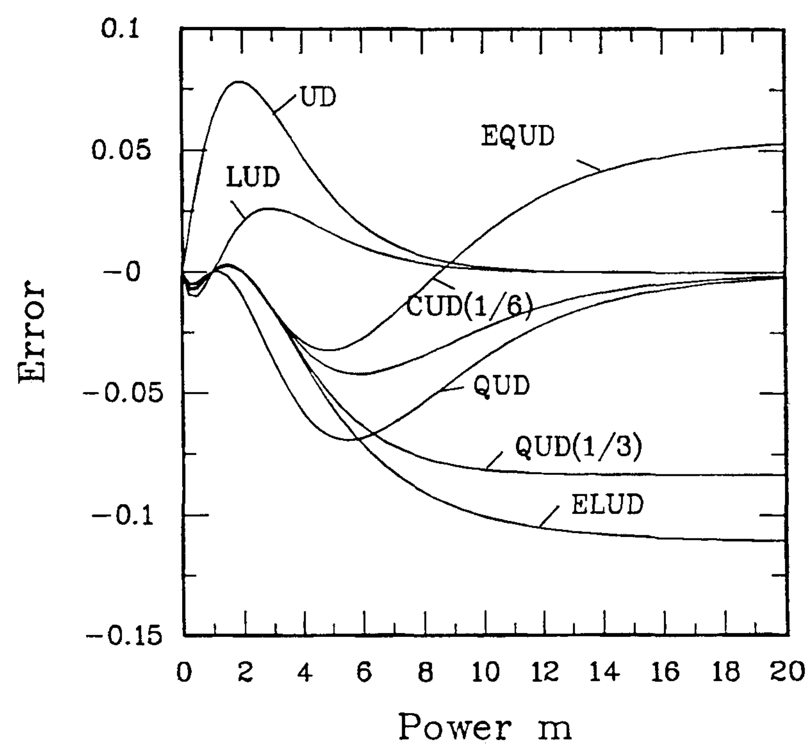


Figure 4. Variation of solution error with power for various schemes for the 1D single-cell analysis, $\phi=x^{m+1}$

the derivatives in the truncation error E_s given by equation (21) become zero. Similarly, the exact solution is obtained for all the third-order schemes if ϕ is of cubic form ($m=2$). It is also seen from the figure that the predictions by the high-order schemes are more accurate than that by the UD for the power less than about three. When the power becomes sufficiently large, the prediction errors of the UD and the second-order schemes approach zero, but not those of the third-order schemes: the errors produced by the ELUD, CUD($\frac{1}{3}$) and EQUD are $-\frac{1}{9}$, $-\frac{1}{12}$ and $\frac{1}{18}$ respectively. The reason is as follows. When m is large, the analytical values of ϕ are virtually zero at nodal points WW, W, P and E and unity at point EE; thus $\phi_P = A_{EE}\phi_{EE}/A_P = A_{EE}/A_P$. According to Table III the ratio A_{EE}/A_P is zero for the first- and second-order schemes, including the CUD($\frac{1}{6}$), and non-zero for the third-order schemes.

Figure 5 presents the leading nine components of the error E_s for each difference scheme against the power m. The term E_{sum} is the sum of the nine error components. If the power is large enough, all the error components of the UD approach zero, whereas for the high-order schemes the high-order components, in turn, dominate. It is noted that an increase of the power means an increase of the gradient of the solution. Also seen from the figure is that for all the schemes apart from the $n=3$ of the QUD the signs of the even-number error components are opposite to those of the odd-number error components. The two sets of components of the second-order schemes, including the CUD($\frac{1}{6}$), have nearly the same magnitude. When the power m becomes sufficiently large, their counter-contribution to the error results in attenuation of the total errors of the second-order schemes as shown in Figure 4. For the third-order schemes the differences between the magnitudes of the even-number and odd-number error components are substantial. Thus the total errors do not decay with an increase of m. It is emphasized here that the error E_{sum} shown in the figure is a sum of truncated errors. It cannot represent the actual error when the power is larger than about 12 because the error components with order higher than 10 have been too large to be ignored.

6.2. Two-dimensional analysis

The case considered here is the two-dimensional convection problem given by equation (23) in the region $-0{\cdot}5 \le x, y \le 0{\cdot}5$. By assuming the flow to be uniform, ϕ is independent of the streamline co-ordinate ξ, as shown by equation (24). It is assumed that

$$\phi = (1+\eta)^m, \tag{33}$$

where η is the co-ordinate normal to the streamline co-ordinate. The origin of the co-ordinates is set at the central point. Thus the analytical solution is $\phi_P = 1$. The effect of flow angle on the numerical solution for different powers is illustrated in Figure 6. For a quadratic distribution ($m=2$) all the difference schemes except the UD give the exact solution (Figure 6(a)) because all the derivatives of the cross-stream truncation error E_c given by equation (26) vanish. Similarly, the calculations of the third-order schemes are free from error for $m=3$ (Figure 6(b)). Figure 6(c) presents the results for $m=9$. Generally speaking, the UD scheme has larger cross-stream error for all flow angles. All the schemes give error-free solutions at 0° flow angle and have the largest errors at 45° angle. The LUD is the most accurate and the QUD the most unfavoured scheme. However, for another case

$$\phi = (1-\eta)^9, \tag{34}$$

shown in Figure 7, the situation is somewhat different. The QUD stands the best while the LUD is the most unpreferred. Besides, the largest cross-stream errors occur at about 22·5° flow angle for the high-order schemes and about 35° angle for the UD scheme.

Figure 8 displays the variation of the error components of the cross-stream truncation error E_c with flow angle for the case $\phi = (1+\eta)^9$. The odd-number error terms vary like sinusoidal

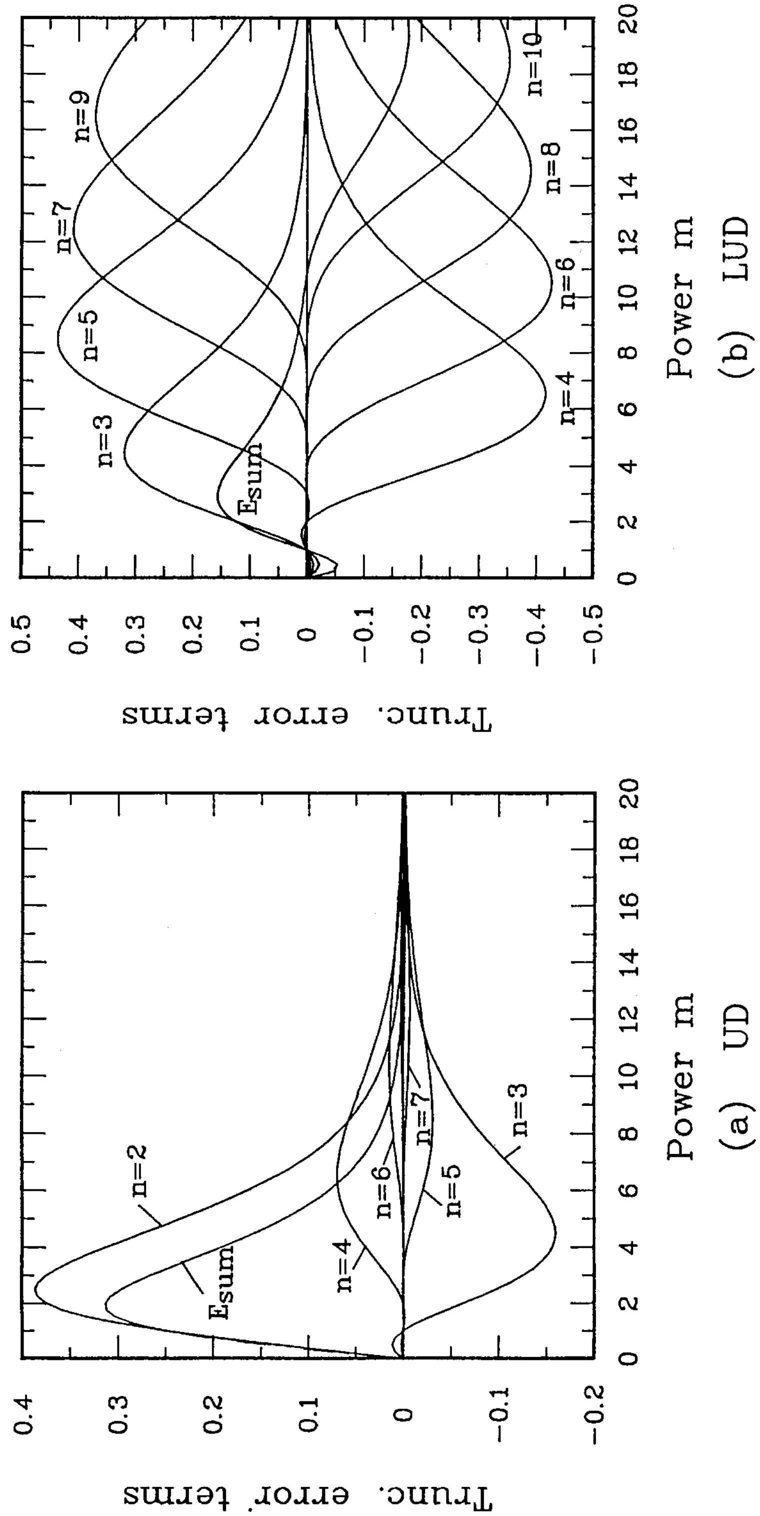


Figure 5. Variation of leading truncation error terms with power for various schemes for the 1D single-cell analysis, $\phi = x^{m+1}$: (a) UD; (b) LUD; (c) QUD; (d) ELUD; (e) CUD($\frac{1}{3}$); (f) CUD($\frac{1}{6}$); (g) EQUD

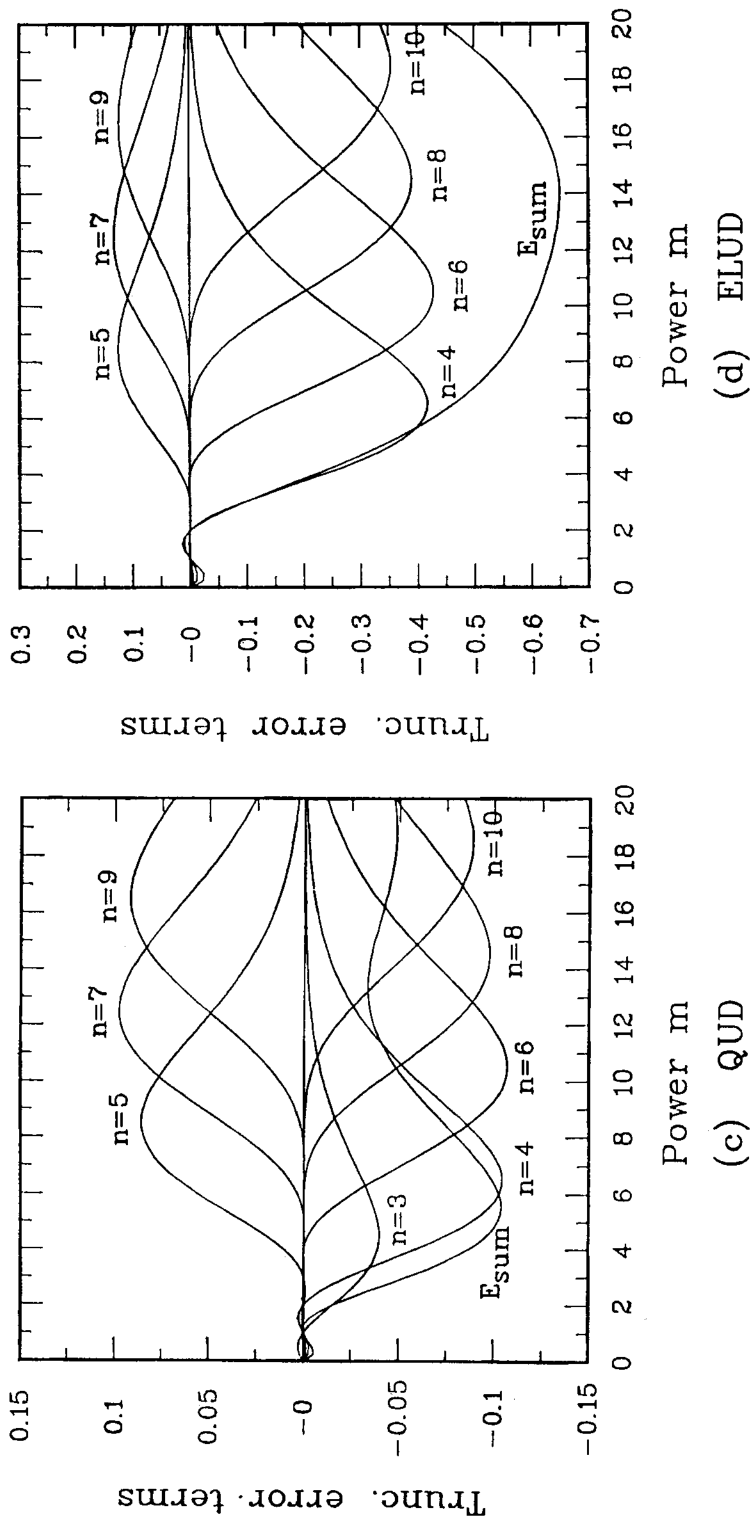
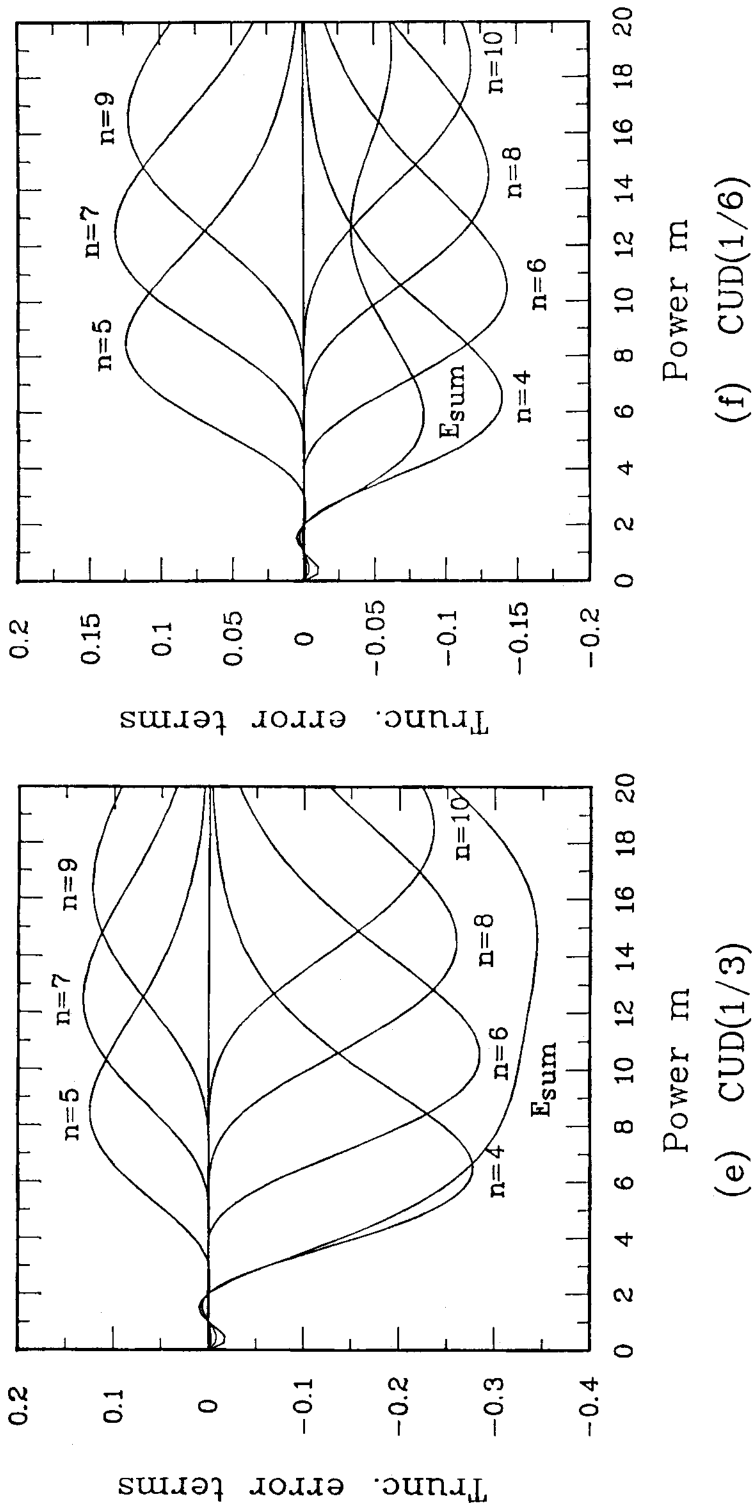


Figure 5 (Continued)



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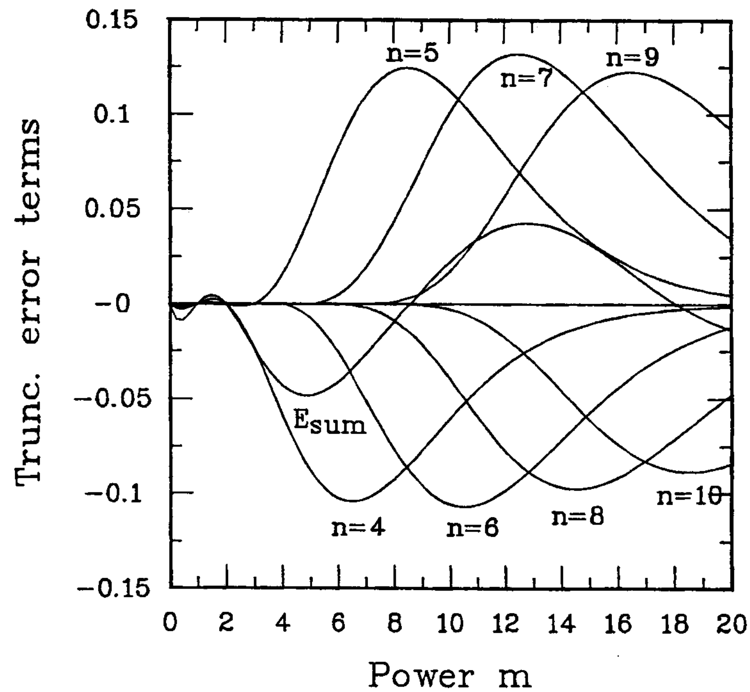


(g) EQUD

Figure 5 (Continued)

functions with their peaks at 22·5° flow angle. The even-number errors increase almost monotonically with the flow angle. Since the odd-number and even-number errors have different signs ($n=3$ for the QUD is exceptional), they make counter-contributions to the total errors. In contrast, for the case $\phi=(1-\eta)^9$, not shown here, the signs for the two sets of errors are of the same family; their contributions to the total errors are additive.

7. MODEL TEST PROBLEMS

The analysis in the last section was limited to a single point. All the errors of the solution are attributed to the truncation error of the discretization. In actual calculations the domain of solution is partitioned into a number of cells. Any error produced at one point will propagate and affect the other points. The single-cell analysis does not reflect the effects of error propagation and accumulation. In order to evaluate the difference schemes, tests must be performed over a representative mesh. The problems chosen here are one- and two-dimensional linear transport equations with or without sources, for which the analytical solutions are available. Solutions of these model problems are obtained using the PDMA (penta-diagonal matrix algorithm), which is an extension of the TDMA (tri-diagonal matrix algorithm). It is a direct solver when applied to one-dimensional cases. For the two-dimensional cases a line-by-line relaxation is used to sweep across the whole domain in an alternating direction manner. In the following the CD is excluded from the study.

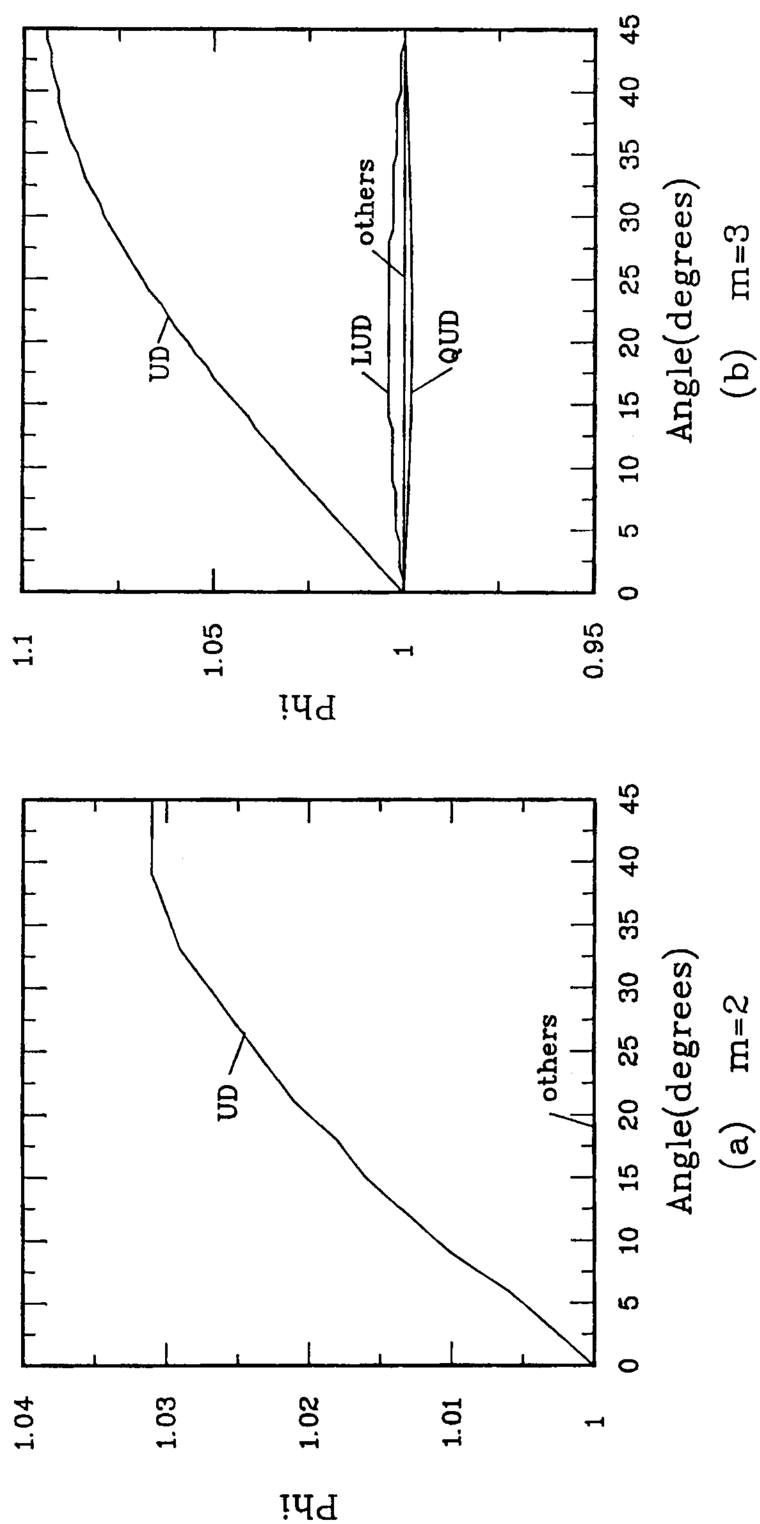
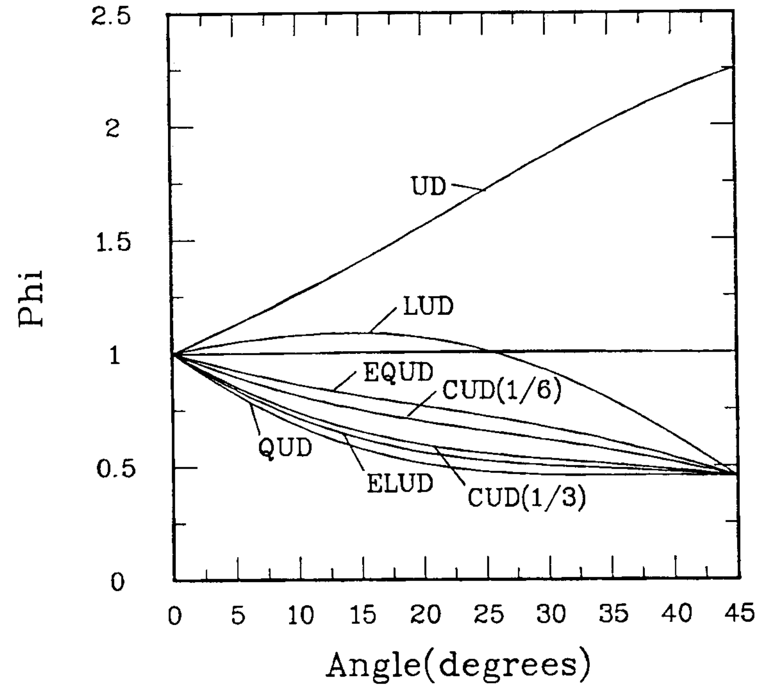


Figure 6. Variation of solution error with flow angle for various schemes for the 2D single-cell analysis, $\phi = 1(1+\eta)^m$: (a) $m=2$; (b) $m=3$; (c) $m=9$



(c) m=9

Figure 6 (Continued)

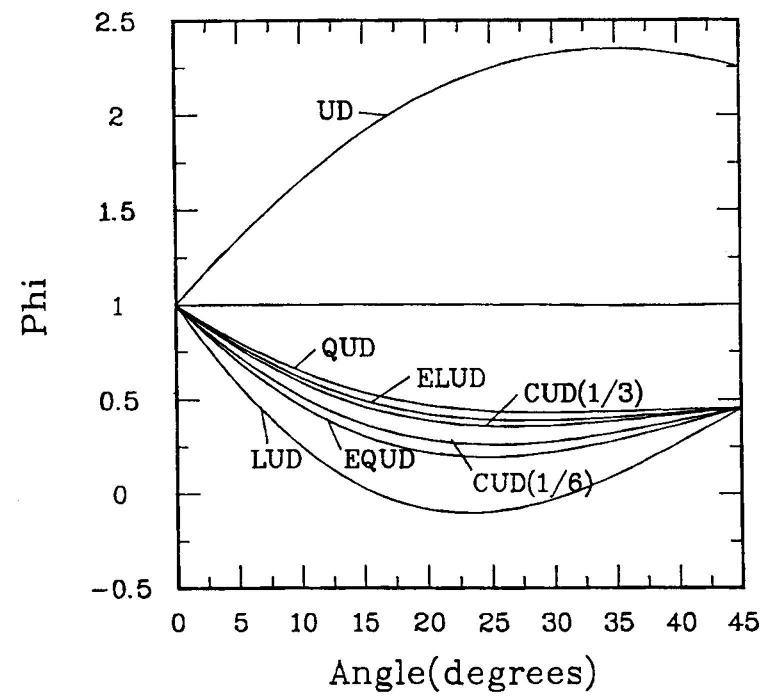


Figure 7. Variation of solution error with flow angle for various schemes for the 2D single-cell analysis, $\phi=(1-\eta)^9$

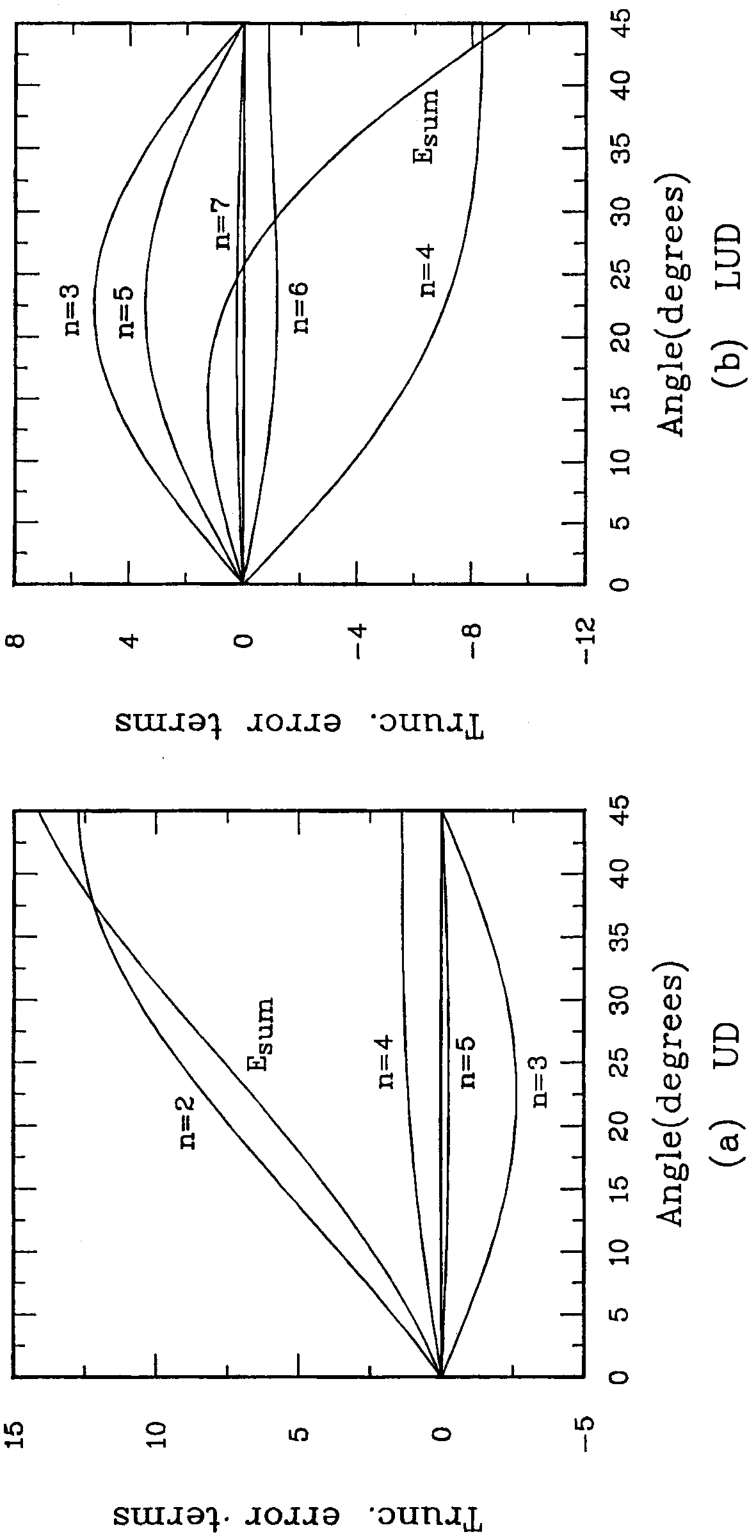


Figure 8. Variation of leading truncation error terms with flow angle for various schemes for the 2D single-cell analysis, $\phi=(1+\eta)^9$: (a) UD; (b) LUD; (c) QUD; (d) ELUD; (e) CUD($\frac{1}{3}$); (f) CUD($\frac{1}{6}$); (g) EQUD

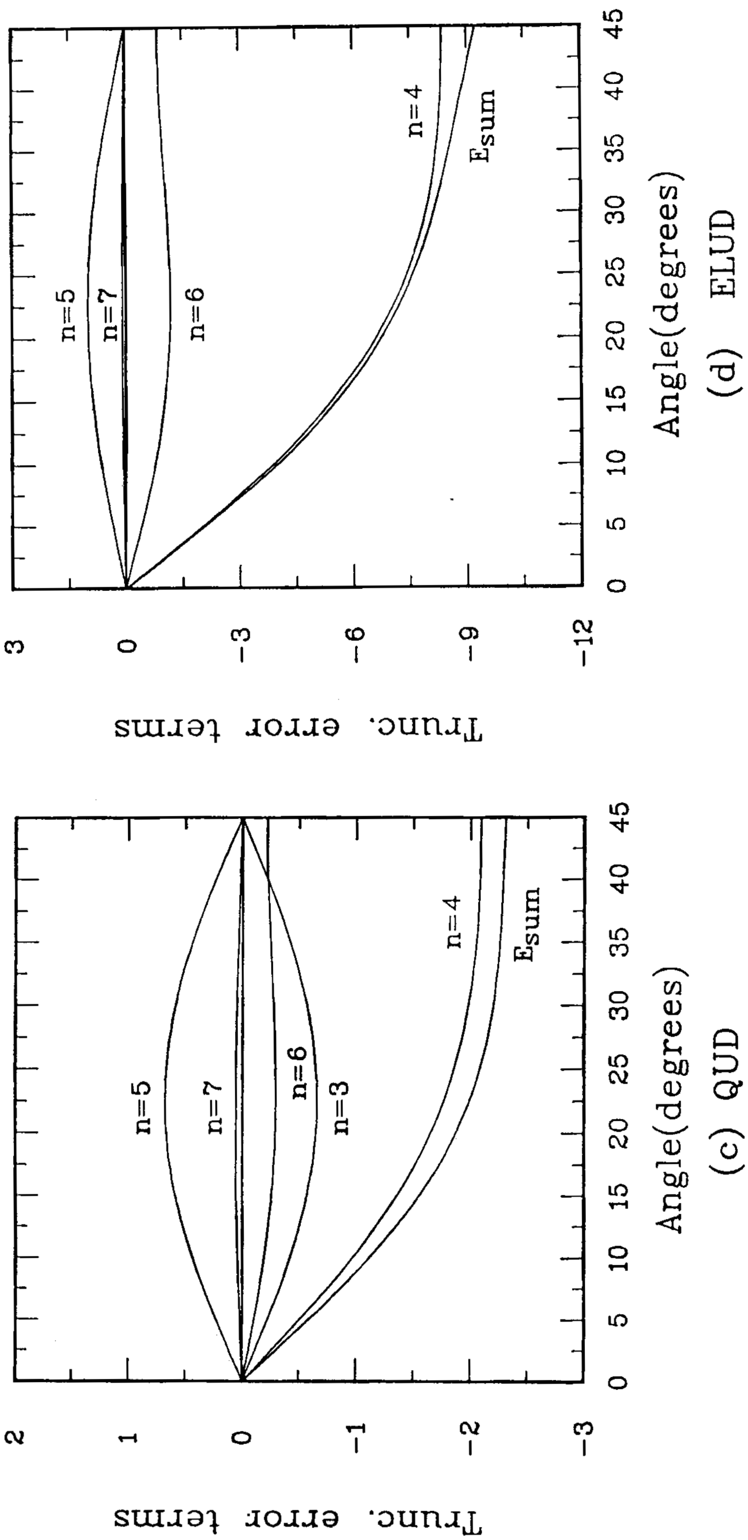
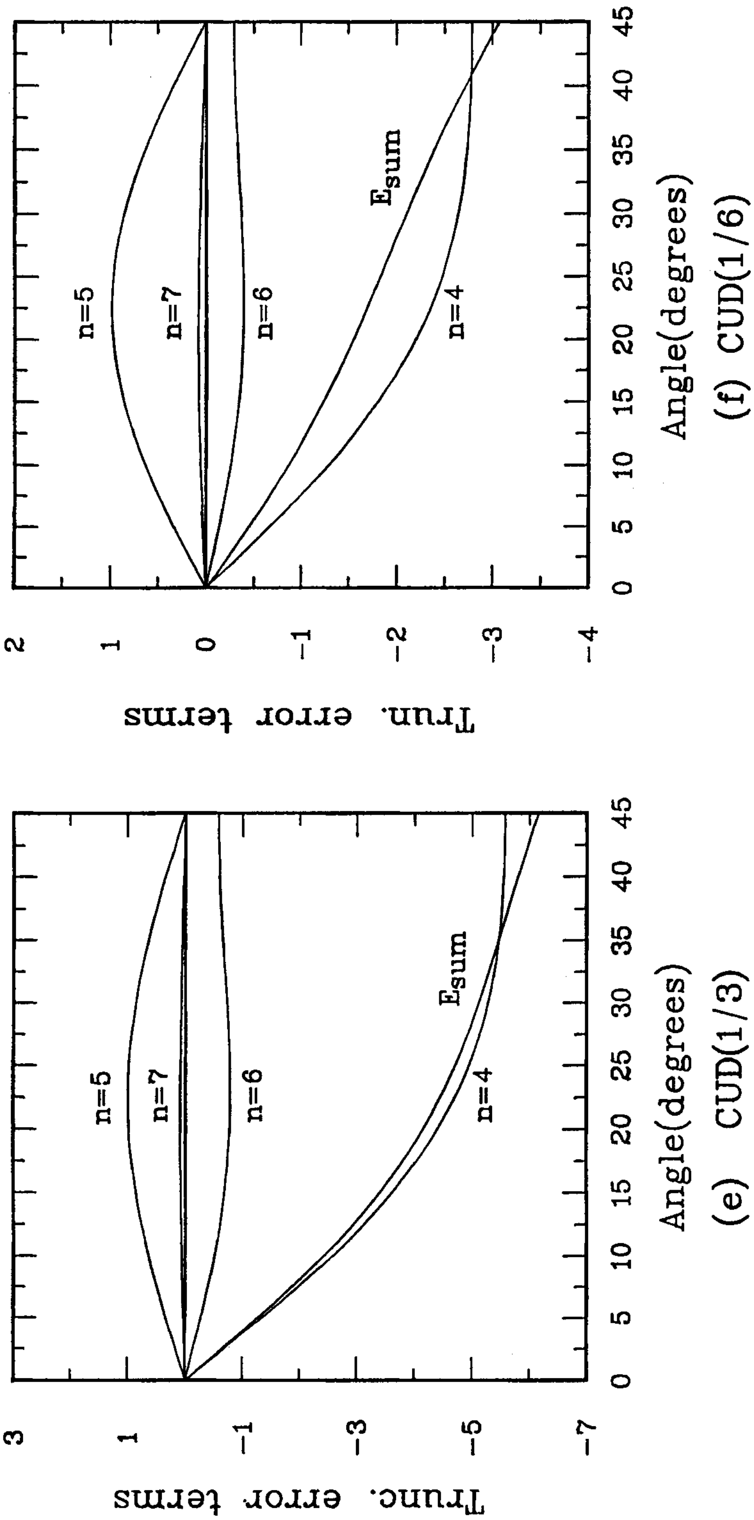


Figure 8 (Continued)



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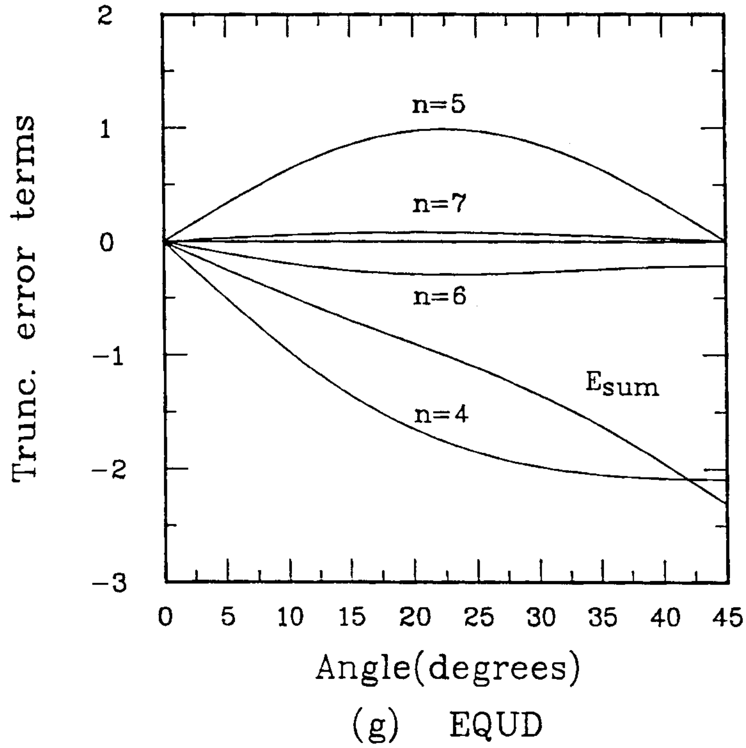

Figure 8 (Continued)

7.1. One-dimensional model cases

The steady one-dimensional transport equation has the form

$$u\frac{d\phi}{dx}=\Gamma\frac{d^2\phi}{dx^2}+S, \quad 0\leq x\leq 1. \tag{35}$$

Three test cases are examined.

Case I: Convection and diffusion in absence of source. This case is subject to the boundary conditions $\phi=0, 1$ at $x=0, 1$ respectively. The analytical solution is obtained as

$$\phi=\frac{1-\exp(Px)}{1-\exp(P)}, \tag{36}$$

where $P=u/\Gamma$ is the Peclet number of the flow. This case has been widely used for testing difference schemes. The computational domain is divided into five cells. Figure 9 shows the results for Peclet numbers $P=10$ and 50, i.e. for cell Peclet numbers $Pe=2$ and 10. When the Peclet number, or more precisely the cell Peclet number, is small, the high-order schemes yield better results, as shown in Figure 9(a). However, undershoots can be seen in the solutions by the ELUD and CUD($\frac{1}{3}$). As the Peclet number increases, the oscillations become prominent in the solutions of all the schemes except the UD and LUD. The solutions by the QUD and EQUD are most unacceptable owing to serious spurious oscillations.

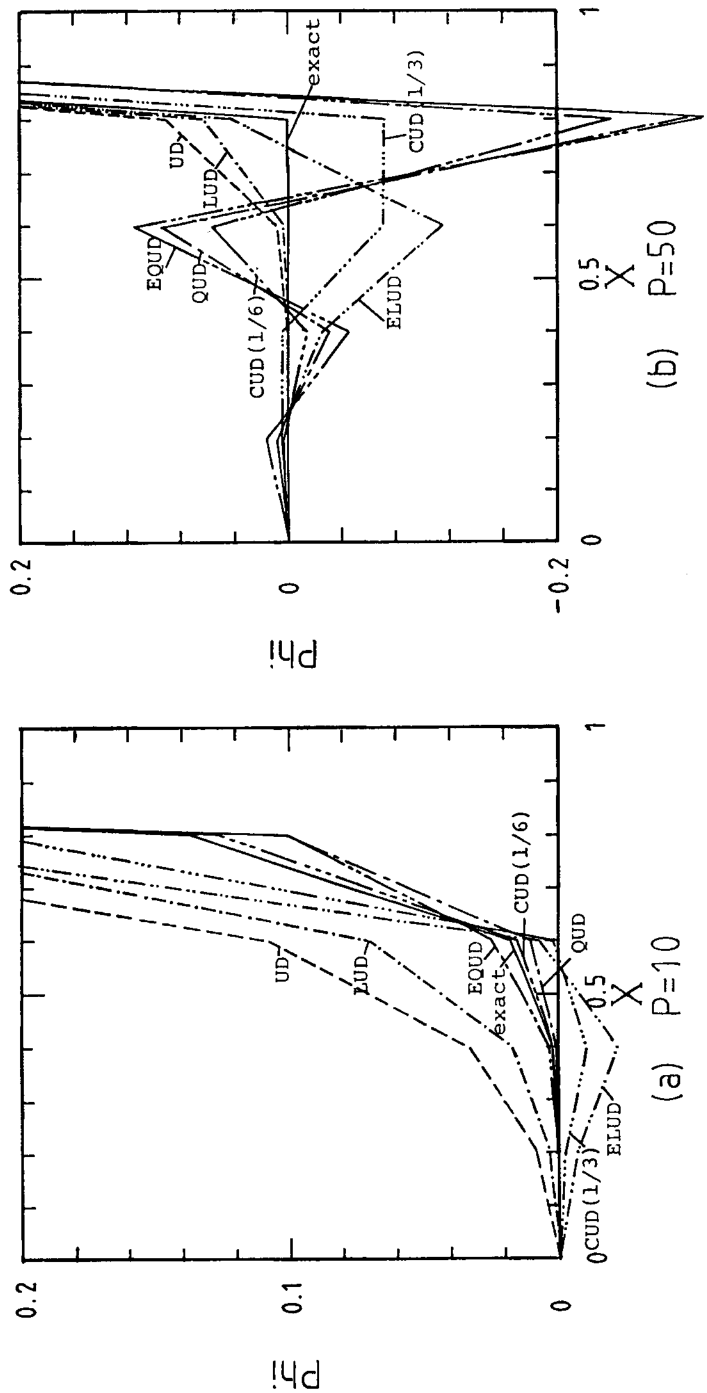

Figure 9. Comparison of calculations by various schemes for the 1D convection/diffusion model case: (a) $P = 10$; (b) $P = 50$

Case II: Convection with plane source (without diffusion)

$$S=\begin{cases}1 & \text{at } x=0{\cdot}5,\\ 0 & \text{elsewhere.}\end{cases} \tag{37}$$

The analytical solution is

$$\phi=\begin{cases}0 & \text{for } x<0{\cdot}5,\\ 1 & \text{for } x\geq 0{\cdot}5.\end{cases} \tag{38}$$

This case was employed by Syed *et al.*[18] to evaluate the QUD and CUD($\frac{1}{6}$). Figure 10 shows the results of the present calculations for $\Delta x=0{\cdot}1$. The UD yields the exact solution and the LUD underpredicts after the mid-length of solution domain. The solutions by the other schemes exhibit oscillations in the first half of the computational domain and similar behaviour to that of the LUD in the other half. It is interesting to note that the shapes of the oscillations are very similar to those in Figure 9(b) for the case of pure convection and diffusion with large Peclet number.

Case III: Convection with linear source (without diffusion)

$$S=\begin{cases}-80x+24, & 0\leq x\leq 0{\cdot}4,\\ 80x-40, & 0{\cdot}4\leq x\leq 0{\cdot}5,\\ 0, & x\geq 0{\cdot}5.\end{cases} \tag{39}$$

The analytical solution is

$$\phi=\begin{cases}-40x^2+24x, & 0\leq x\leq 0{\cdot}4,\\ 40x^2-40x+12{\cdot}8, & 0{\cdot}4\leq x\leq 0{\cdot}5,\\ 2{\cdot}8, & x\geq 0{\cdot}5.\end{cases} \tag{40}$$

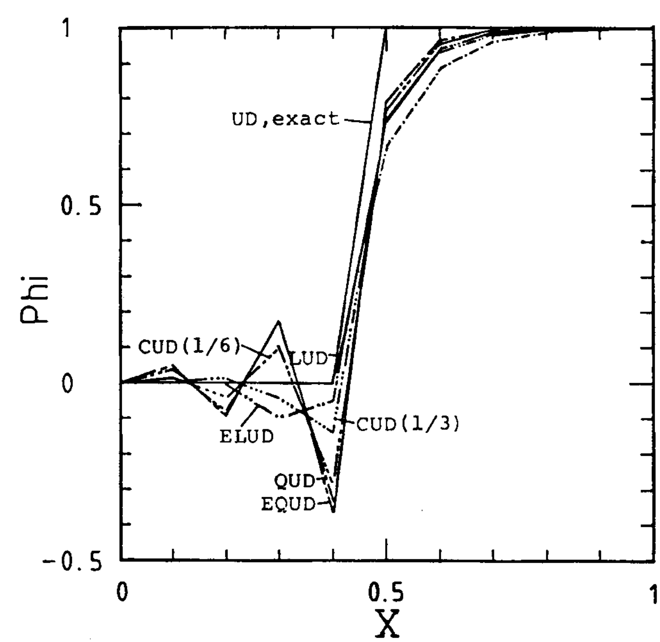

Figure 10. Comparison of calculations by various schemes for the 1D convection model case with plane source

This kind of model problem has been chosen by Leonard[8] and Shyy[16] to evaluate the QUD and LUD schemes. From the results shown in Figure 11 it is obvious that the UD computation has substantial error while the solutions by the high-order schemes are close to the exact one, with the LUD being the best. It has been shown by Leonard[8] that the UD prediction for this case is identical to the CD computation for the convection/diffusion case with cell Peclet number $Pe=2$ owing to the fact that the artificial viscosity $\Gamma=u\Delta x/2$ is embedded in the UD scheme.

7.2. Two-dimensional model cases

The two-dimensional convection/diffusion transport equation is given as follows:

$$u\frac{\partial \phi}{\partial x}+v\frac{\partial \phi}{\partial y}=\Gamma\left(\frac{\partial^2 \phi}{\partial x^2}+\frac{\partial^2 \phi}{\partial y^2}\right). \tag{41}$$

Here two cases are considered.

Case IV: Convection of a step discontinuity in a uniform flow. This model problem was first used by Raithby[5,28] and then widely employed to test the cross-stream numerical diffusion of difference schemes. In this case the diffusion terms are neglected and the flow is assumed uniform at an angle θ to the x-axis. This equation can be reduced to

$$\frac{\partial \phi}{\partial x}+\tan\theta\frac{\partial \phi}{\partial y}=0. \tag{42}$$

The analytical solution is that ϕ is constant along each streamline. Thus the solution is equal to the inlet value, which is a function of the co-ordinate normal to the streamlines. By assuming the

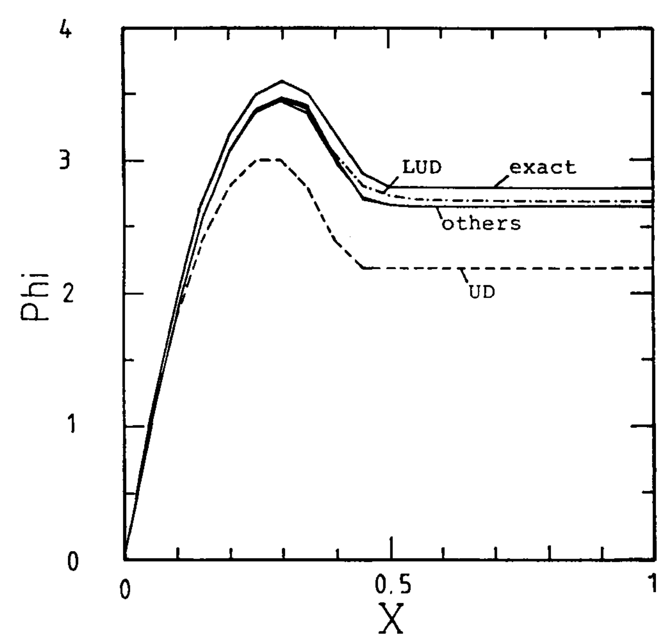

Figure 11. Comparison of calculations by various schemes for the 1D convection model case with linear source

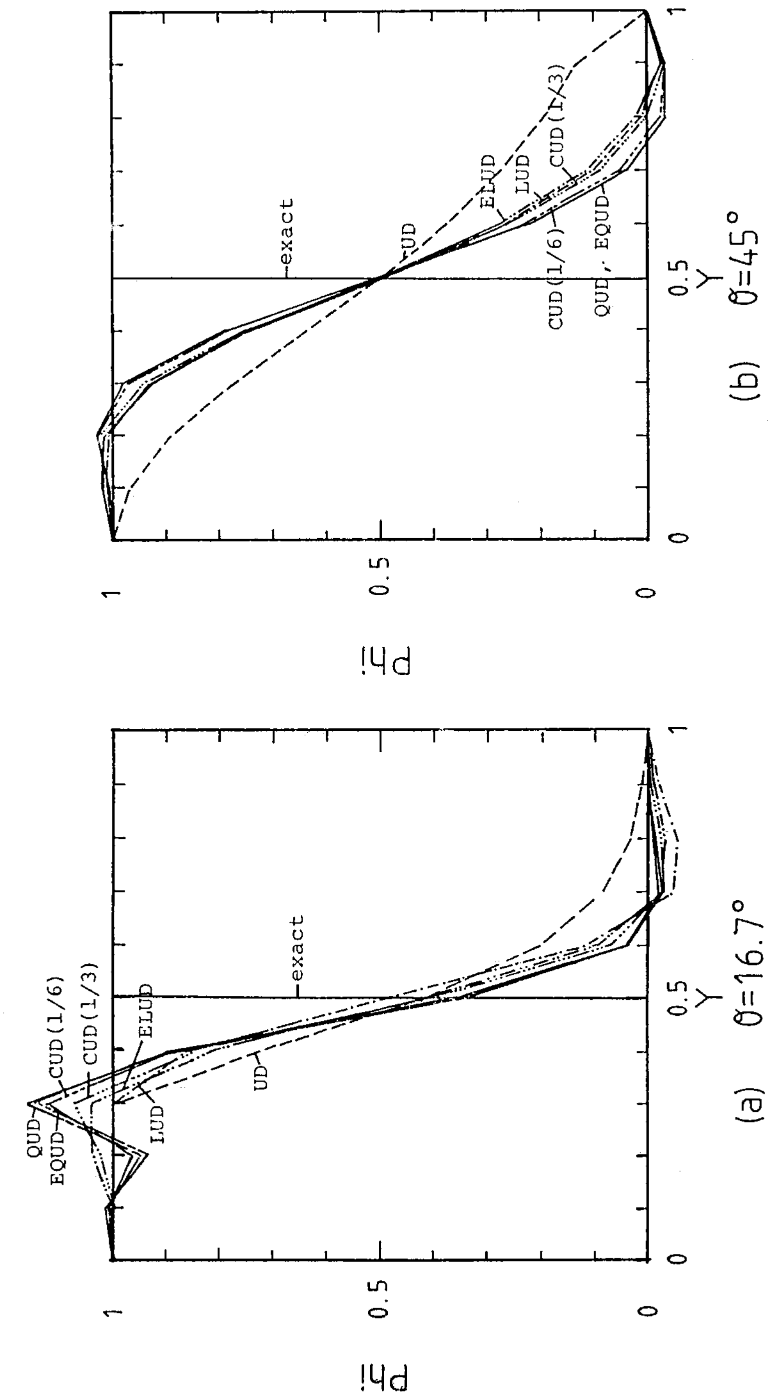

Figure 12. Comparison of calculations by various schemes for the 2D convection model case with uniform flow: (a) $\theta = 16{\cdot}7°$; (b) $\theta = 45°$

convected inlet value to be a step function, in inlet boundary conditions are specified as

$$\phi=\begin{cases}0 & \text{at } y=0,\ 0\le x\le 1 \text{ and } x=0,\ 0\le y<y_0,\\ 1 & \text{at } x=0,\ y_0<y\le 1,\end{cases} \tag{43}$$

where

$$y_0=\frac{1-\tan\theta}{2}. \tag{44}$$

The results at the mid-plane ($x=0{\cdot}5$) are shown in Figure 12 for $\theta=16{\cdot}7°$ and 45°. The large numerical diffusion of the UD results in a large smearing error when compared with the high-order schemes. However, overshoots and undershoots cannot be avoided in the solutions of the high-order schemes. Similar to the results in the one-dimensional flow, the QUD and EQUD have the largest unboundedness problem but the steepest gradients. Comparing Figures 12(a) and 12(b) reveals that as the flow angle increases, the solution becomes flatter and the oscillatory behaviour is less obvious for all the schemes owing to the increasing cross-stream diffusion.

Case V: Convection and diffusion of a step discontinuity in a recirculating flow. This problem was devised by Smith and Hutton[15] in a meeting to evaluate more than 20 different numerical schemes. It has been adopted by Runchal[29] to evaluate his CONDIF method. This test problem retains an important feature of the recirculating flow: the streamline curvature. A schematic diagram of the problem is illustrated in Figure 13. The governing equation is given by equation (41). The velocity components are prescribed as

$$u=2y(1-x^2), \tag{45a}$$

$$v=-2x(1-y^2). \tag{45b}$$

The boundary conditions on the east, west and north faces of the domain of solution are prescribed as

$$\phi=1-\tanh C \quad \text{at } x=\pm 1,\ 0\le y\le 1 \text{ and } y=1,\ -1\le x\le 1. \tag{46}$$

The inlet condition at the south face is

$$\phi=1+\tanh[(2x+1)C] \quad \text{at } y=0,\ -1\le x\le 0. \tag{47}$$

In the above the constant C is taken to have the value 10. Thus ϕ is essentially zero on the 'solid' boundaries and a step profile with $\phi=0$ for $x<-0{\cdot}5$ and $\phi=2$ for $x>-0{\cdot}5$ at the inlet boundary.

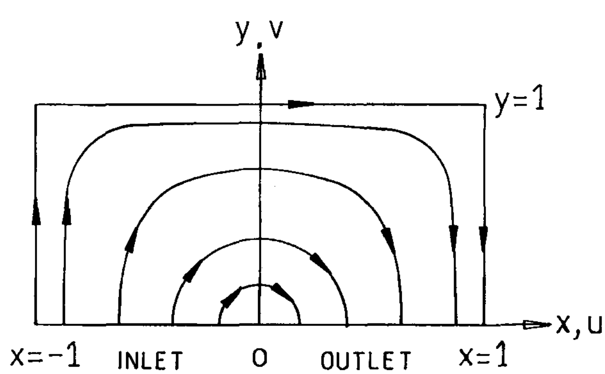

Figure 13. Schematic illustration of the 2D recirculating flow problem

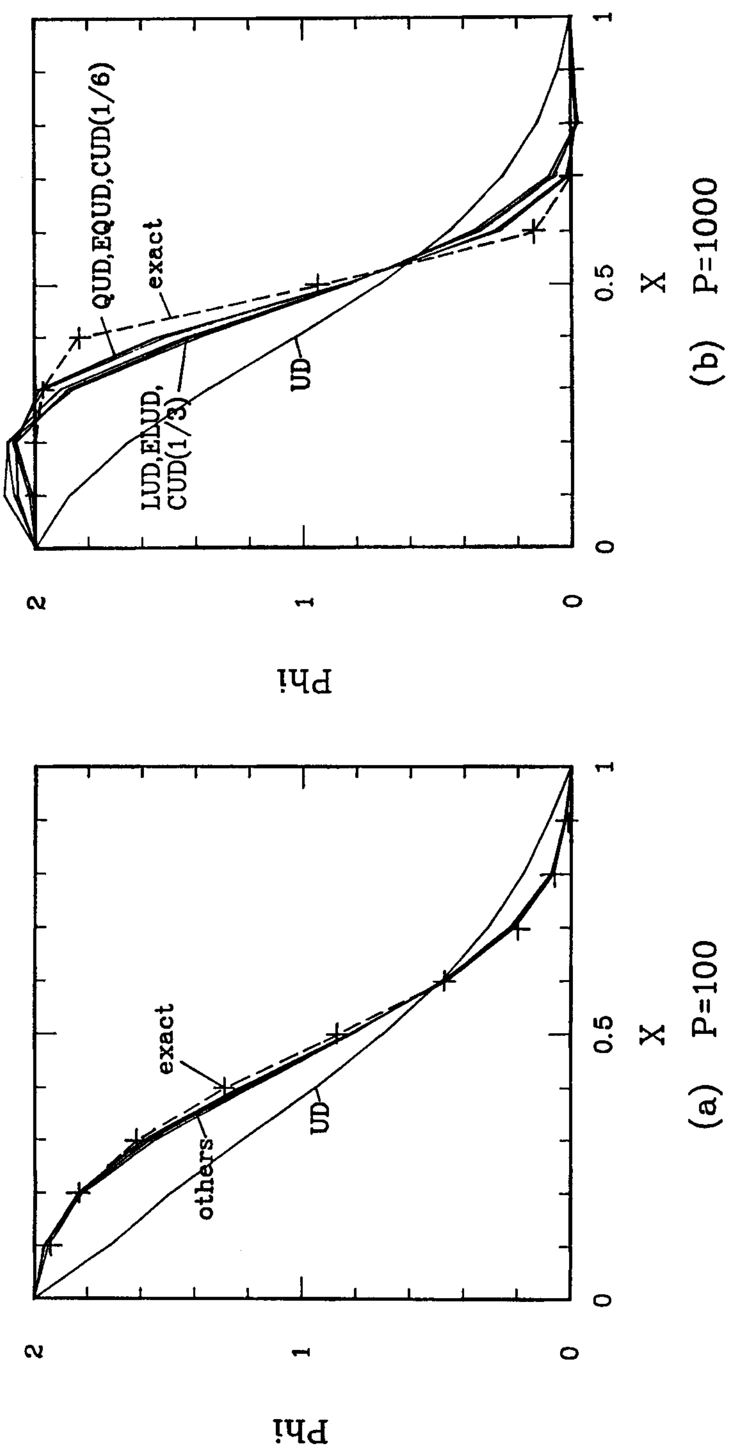

Figure 14. Comparison of calculations by various schemes for the 2D recirculating flow model case for $\Delta x = \Delta y = 0{\cdot}1$: (a) $P = 100$; (b) $P = 1000$

At the outlet the zero-gradient condition is imposed. The computational domain is divided into 20×10 cells with mesh interval $\Delta x = \Delta y = 0{\cdot}1$. The ϕ-distributions by the difference schemes for flow Peclet numbers $P = 100$ and 1000 are shown in Figure 14. Also show in the figure are a set of numerical data which are used by Smith and Hutton as representative of the exact solution. Again it demonstrates the prevailing of the numerical diffusion for the UD scheme. For the low-Peclet-number case the solutions by the high-order schemes agree well with the exact solution. When the Peclet number is increased to $P = 1000$, the calculations show substantial differences from the exact one. Besides, overshoots and undershoots appear in the solutions. To improve the accuracy, the mesh is refined to give $\Delta x = \Delta y = 0{\cdot}05$. As shown in Figure 15, the results obtained by the high-order schemes are close to the exact solution in the region of steep gradient. The amplitudes of the wiggles are also much reduced.

8. CONCLUSIONS

Analysis and evaluation have been performed on a general difference scheme which represents a number of first-, second- and third-order schemes. The main conclusions can be drawn as follows.

1. Examination of the coefficients of the difference schemes shows that it is impossible to get rid of negative coefficients for the upstream-weighted high-order schemes and thus unboundedness cannot be avoided in the solutions by these schemes.
2. The formal order of accuracy cannot ascertain the accuracy of a given scheme because the high-order terms in the truncation error may dominate the error when the gradient of the solution is steep.

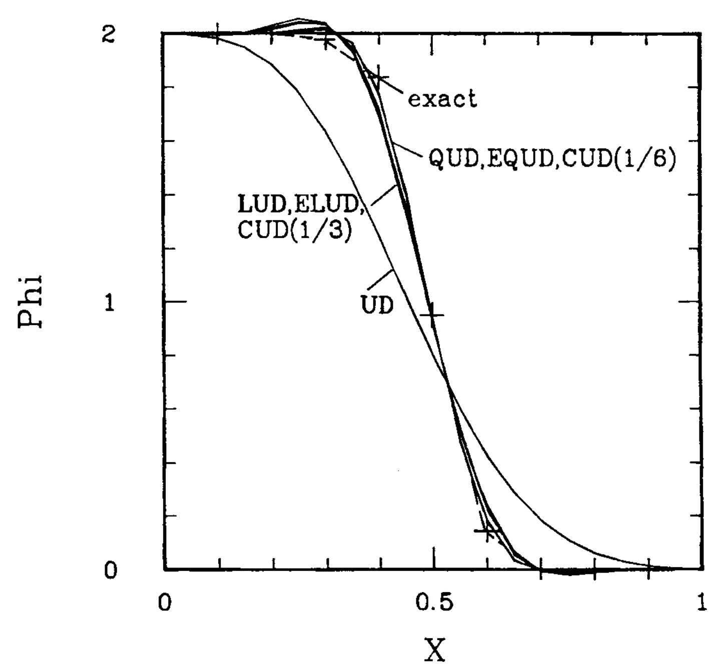

Figure 15. Comparison of calculations by various schemes for the 2D recirculating flow model case for $P = 1000$ and $\Delta x = \Delta y = 0{\cdot}05$

3. Each of the upstream-weighted high-order schemes can be regarded as a non-dissipative five-point central difference with a fourth-order numerical dissipation. The fourth-order dissipation is not able to smear out the high-frequency errors. This confirms the previous conclusion that it is impossible for these schemes to suppress oscillations.
4. In the choice of the high-order schemes the LUD scheme show the best compromise between numerical diffusion and unboundedness. The solutions of the QUD and EQUD suffer from the largest oscillations. According to our experience with use of the PDMA as the solution solver in solving two-dimensional cases, the LUD is the most cost-effective, while the QUD and EQUD require the largest underrelaxation during the solution iteration and thus much more computer time.

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