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DISCUSSION ON NUMERICAL STABILITY AND BOUNDEDNESS OF CONVECTIVE DISCRETIZED SCHEME

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Existing methods for analyzing the stability of a discretized scheme for convection-diffusion terms are usually based on five assumptions, i.e., one-dimensional, linear, first kind of boundary condition, source term free, and uniform grid system. In this article we examine numerically whether deviation from one of the assumptions may enhance the stability of the discretized scheme. The second part of the article is devoted to the criterion of convective boundedness. It is shown that the convective boundedness criterion (CBC) proposed by Gaskell and Lau is only a sufficient condition. Another region in the normalized variable diagram is proposed within which any scheme defined is convectively bounded. Three new bounded high-resolution schemes defined in this region, SBECBC1, 2, and 3, are proposed, and numerical experiments for two advection problems and one diffusion-convection problem demonstrate the high-resolution ability of the SBECBCs for a sharp change in scalar profile.

INTRODUCTION

Successful simulation of convection is one of the most challenging and interesting research branches in computational fluid dynamics (CFD) and numerical heat transfer (NHT), which attracts many CFD/NHT workers to exert themselves to develop an ideal (perfect) scheme. It is well known that stability, boundedness, and accuracy are the most important properties of modeling schemes for the convection term. In developing a computational program for fluid flow and heat transfer problems it is desired to adopt a modeling scheme possessing high accuracy, high stability, and boudedness characteristics with reasonable computational effort. In practice, however, no scheme has been proved to have such virtues simultaneously. The difficulty in devising a satisfactory scheme lies in the conflicting requirements of accuracy on one hand, and stability and boundedness on the other. High-order-accuracy schemes may lead to unphysical oscillatory or overshoot/undershoot behavior in the region where steep gradients exist, while computations based on classical first-order upwind schemes (FUS) or the like often suffer severe inaccuracies

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NOMENCLATURE

A	coefficients of the discretized equation Superscripts
f	cell face
I	total flux across the cell face
Q	source term in transport equation
S	source term in the discretized equation
u	velocity component in x direction
v	velocity component in y direction
$\mathbf{U}$	velocity vector
Γ	diffusion coefficient
ρ	density
ϕ	general dependant variable

Superscripts

C	convection contribution
D	diffusion contribution

Subscripts

A	refers to deferred correction
C	central grid point
D	downstream grid point
E, W, N, S	refer to neighbors of the P grid point
e, w, n, s	refer to the control-volume face
f	refers to the control-volume face
NB	refers to neighbors
P	main grid point
U	upstream grid point

due to the so-called false diffusion resulting from low-order truncation error. It is widely accepted that the central difference scheme (CDS) is a conditionally stable scheme owing to its small critical Peclet number, over which the numerical results may be oscillating [1–4]. However, many recent studies [5–7] using the central difference scheme show that numerical solutions resulting from the central difference scheme are often found to have no oscillatory behavior, though the grid Peclet number is much greater than the critical Peclet number 2, obtained from the analysis of a one-dimensional model equation. Recently, research work [8–10] again revealed a similar phenomenon. For example, the numerical results in [10] show that for the case of impingement heat transfer of oncoming flow onto slatlike surfaces, the central difference scheme for the convection term still leads to a physically reasonable solution, even though in most computational regions the grid Peclet number is much greater than 2, with the maximum Peclet number as high as 180. To the best of the authors' knowledge, there seem to be no articles in the literature which indicate clearly the reasons for such different results from the classic analysis [1–4]. It is to be noted that conventionally the stability analysis for the discretized convection-diffusion equation is conducted for one-dimensional, linear, source-free, and two-point boundary-value problems on a uniform grid system. Thus, one purpose of the present study is to reveal the effect on the critical grid Peclet number if one of the above-mentioned five conditions is not fulfilled. The terminology of critical Peclet number is adopted here to represent that value of grid Peclet number beyond which wiggles will occur in the numerical solution.

Another important property of convective schemes, boundedness, is also studied in this article. When the convection term is discretized by a bounded scheme, the resulting numerical solution will never surpass the maximum or minimum values inherently determined by the physical process itself. For example, the concentration of a component of a mixture can only be varied from 0 to 1. If the numerical results of concentration from some convection scheme have local values larger than 1 (overshoot) or less than 0 (undershoot), the convection scheme does not possess boundedness. Obviously, boundedness is of immense importance to keep numerical results physically reasonable, especially for the case where a large gradient occurs in

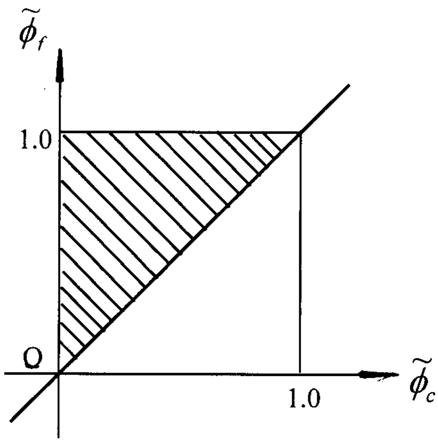


Figure 1. Gaskell and Lau CBC area in NVD.

the computation domain. Gaskell and Lau [12] proposed a criterion for a convection scheme to possess the boundedness character and named the criterion the convective boundedness criterion (CBC). In addition, they also delineated a corresponding region in the normalized variable diagram (NVD), shown in Figure 1 by the hatched lines. They claimed that the characteristic lines (i.e., the definition line) of all bounded schemes should be located within this region, and vice versa. Considerable efforts have been made in recent years to develop what is called high-resolution composite schemes to overcome the unphysical overshoot/undershoot behavior of some high-order schemes such as QUICK [13]. A number of high-resolution composite schemes have been proposed for the calculation of viscous fluid flow with finite-volume methods. The schemes are, for example, MUSCL [14], CLAM [15], OSHER [16], MINMOD [17], SMART [12], STOIC [18], etc., which all satisfy the convection boundedness criterion. The CBC and the restricted region at the NVD have long been accepted as both sufficient and necessary conditions for a scheme possessing boundedness [12,18,19]. In the authors' opinion, however, the CBC proposed by Gaskell and Lau is only a sufficient condition for a scheme to achieve computed boundedness. In this article, another new sufficient condition is proposed.

NUMERICAL DISCRETIZATION OF THE TRANSPORT EQUATION

The two-dimensional diffusion and convection equation is discretized by the finite-volume method [1]. The diffusion term is discretized by linear interpolation (central difference scheme) [1], while the interfacial term is interpolated by various methods, including central difference, QUICK, and high-resolution schemes. To ensure the solution stability of the discretization equation, the implementation of CDS and QUICK is carried out by the deferred correction procedure proposed by Rubin and Khosla [20] as

$$F_f \phi_f = F_f \phi_f^{\text{FUS}} - F_f(\phi_f^{\text{FUS}} - \phi_f)^* \tag{1}$$

where the superscript FUS denotes values obtained using the first-order upwind scheme, ϕ_f represents cell face value computed by the high-order scheme adopted, and * indicates the value of the previous iteration. The final discretized algebraic equation can be written as follows:

$$A_P \phi_P = \sum_{\mathrm{NB}=E,W,N,S} A_{\mathrm{NB}} \phi_{\mathrm{NB}} + S_P + S_A \tag{2}$$

$$S_A = \sum_{f=e,w,n,s} F_f (\phi_f^{\mathrm{FUS}} - \phi_f)^* \tag{3}$$

where A_P and A_{NB} are the convection-diffusion coefficients obtained from the first-order upwind discretization, S_P is the original source term contribution, and S_A is the contribution from the deferred correction. It should be noted that in some articles the function (or virtue) of the deferred correction technique seems to be exaggerated. For example, in [21], after adopting the defer correction technique to the coefficient rearrangement of QUICK, it is claimed that "the coefficients are always positive and now satisfy the requirements for conservativeness, boundedness and transportiveness." From this statement it seems that once the coefficients of the discretization equation are reorganized by the deferred correction technique, any scheme could be absolutely stable and bounded. Our numerical practice does not support such viewpoint. As illustrated in [22], deferred correction is an efficient way to ensure the solution stability of discretization equation, but it cannot change the inherent convective stability and boundedness of a scheme.

STABILITY OF FINITE-DIFFERENCE SCHEME FOR THE CONVECTIVE-DIFFUSION EQUATION

As indicated earlier, all existing analysis methods on the stability of convection-diffusion difference schemes are based on the following five assumptions: (1) one-dimensional; (2) linear; (3) source term free; (4) uniform grid; and (5) two-point boundary-value problem. However, practical problems are often far away from the above assumptions—for example, three-dimensional nonlinear fluid mechanics problems are often encountered in computational fluid dynamics. Thus it is necessary to investigate the influence of dimension, nonlinearity, source term, boundary condition, and nonuniform grid on the stability of different schemes. In the following sections we will demonstrate that all five factors have effects, more or less, on the stability of convection finite-difference scheme.

1. Influence of the Boundary Condition

As stated above, all existing stability analysis methods consider only the first kind, i.e., Dirichlet boundary condition. Leonard studied a one-dimensional problem with such a boundary condition [11]. The one-dimensional equation and boundary condition considered by Leonard took the following form:

$$\rho u \frac{d\phi}{dx} = \Gamma \frac{d^2\phi}{dx^2} + S(x) \qquad x = 0, \phi = 0; \;\; x = 1, \phi = 1 \tag{4}$$

where $S(x)$ is a source term whose variation pattern is shown in Figure 2c.

Leonard discretized the computational domain by practice A [1]. He found that for $P_\Delta = 5$ wiggles appeared at the right end of the computational domain for both the QUICK and central difference schemes. In the present study the same problem

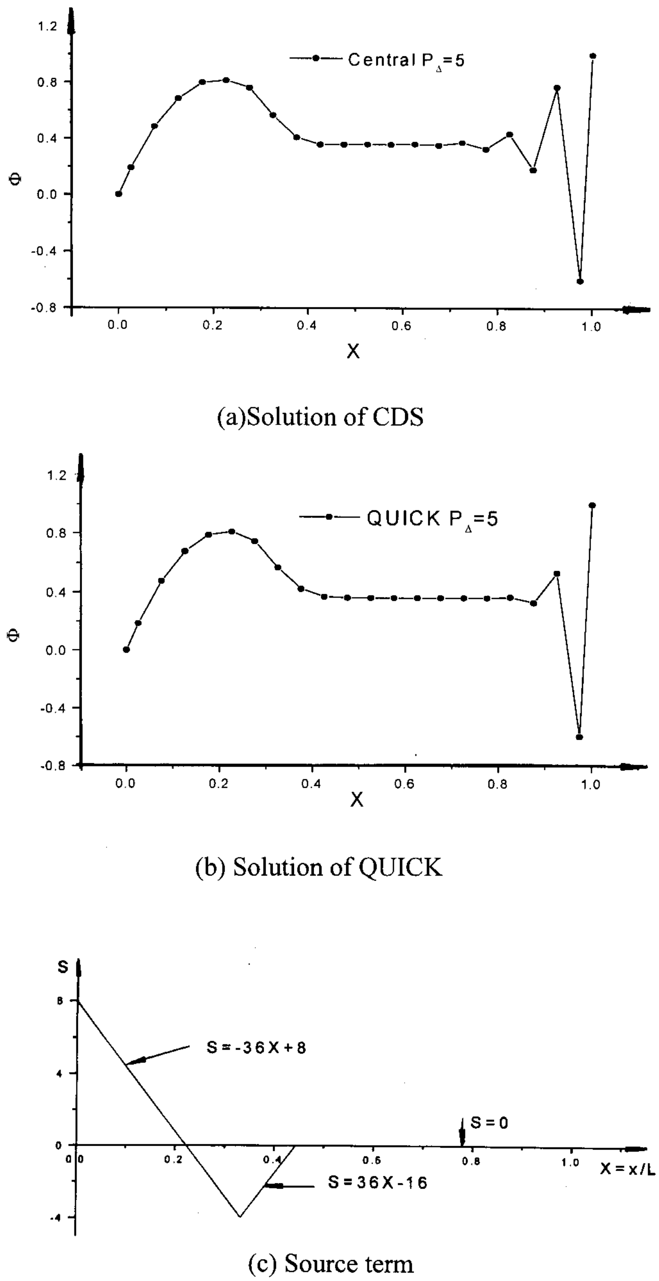


Figure 2. Solution oscillation of CDS and QUICK for $P_\Delta = 5$: (*a*) solution of CDS; (*b*) solution of QUICK; (*c*) source term.

was solved on a grid system resulting from practice B [1] and similar results were observed, with the wiggles caused by the central difference scheme being more severe than those caused by QUICK (see Figures 2*a* and 2*b*). For the same problem, Shyy [23] changed only the boundary condition of the right-hand side from first kind to adiabatic condition, and found that for the QUICK scheme no wiggles occurred even with a Peclet number as high as 10^8. Our computational results also reveal the same phenomenon, which indicates that boundary condition has a great effect on the convective stability.

2. Effect of Nonconstant Source Term in the Entire Domain

A one-dimensional problem with nonconstant source term existing in the entire computational domain (shown in Figure 3*c*) is tested by using both the QUICK and central difference schemes (CDS) with 18 control volumes. The effect of the nonconstant source term seems trivial if the boundary conditions at the two ends are both of first kind, as witnessed from Figures 3*a* and 3*b*, where both QUICK and CDS show oscillatory results when the grid Peclet number is a bit larger than the critical value. However, if the boundary condition of the right-hand side is changed to the third kind, expressed by $\phi_L = \phi_{(L-1)} - 0.1$, then the stability of the two schemes will be greatly enhanced: for QUICK, no oscillation occurs (see Figure 4); for CDS, oscillation does not occur when the grid Peclet number is less than 10 (Figure 5*a*). However, for the case of third-kind boundary condition and zero source term, the solution of CDS is still oscillating (Figure 5*b*). These reuslts illustrate the important influence of both the nonconstant source term and boundary condition on the stability of the convection scheme.

It is interesting to note that Kriventsev and Ninokata [24] recently proposed a so-called EFD scheme in which the convection part is actually upwind-based and the effect of a linearly varied source term was incorporated. Their computational results show that when a linear interpolation cannot describe the source term distribution correctly, EFD may also generate unphysical oscillating solutions even at very high grid Peclet number.

3. Influence of Nonuniform-Grid Peclet Number

The test problem represented by Eq. (4) and Figure 2*c* is adopted again to investigate the influence of nonuniform grid Peclet number. All the conditions are the same as those mentioned in the section on boundary condition influence except the distribution of grid Peclet number. The grid Peclet number in the present problem has different values in the two regions of the computational domain (Figure 6). Grid Peclet number tends to be infinite (diffusive coefficient equals zero) where x is less than $\frac{4}{9}$, while for the rest of the domain, where x is greater than $\frac{4}{9}$, three different values of grid Peclet number are adopted: 0.0556, 0.556, and 5.56, corresponding to three cases. Three curves shown later, in Figure 10, represent the three test cases, which show the influence of nonuniform grid Peclet number distribution on stability. Inspection of the results reveals that: (1) when grid Peclet number equals 0.556, no oscillatory behavior is found; while for grid Peclet numbers 0.0556 and 5.56, wiggles

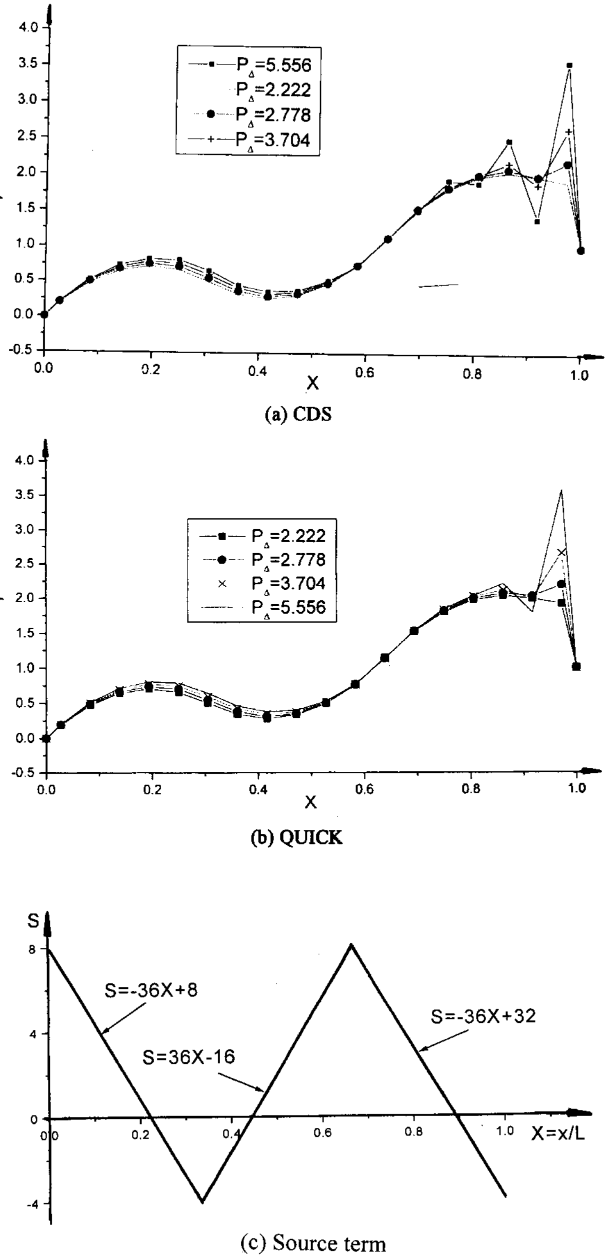


Figure 3. Numerical solutions for first-kind boundary condition with entire-domain-filled source term (CDS and QUICK): (*a*) CDC; (*b*) QUICK; (*c*) source term.

appear; and (2) for the two unstable cases, wiggles occur on different sides of the computational domain, showing that oscillatory behavior may not be just a local phenomenon.

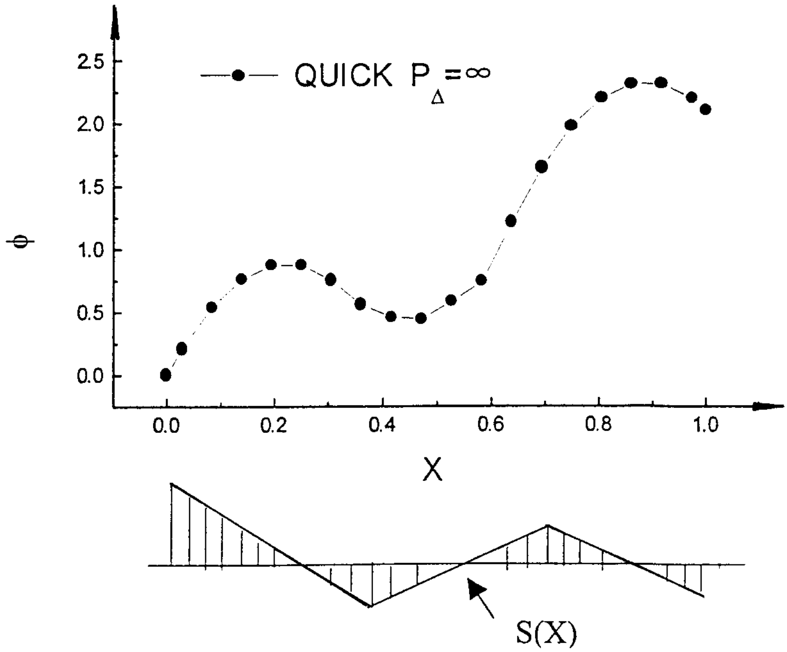


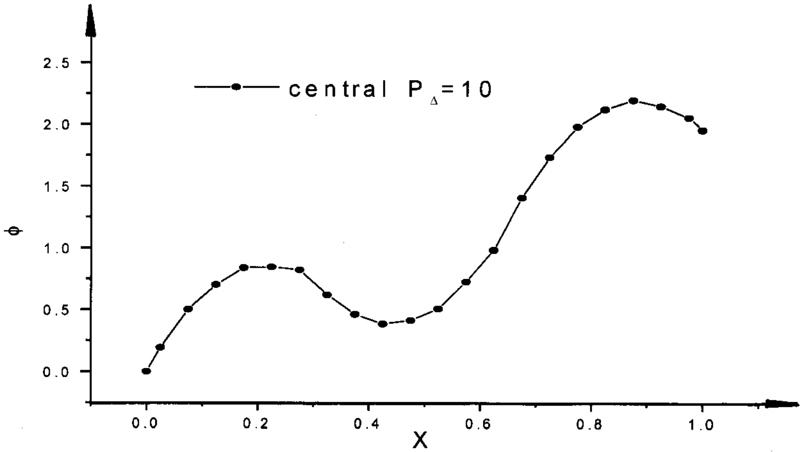
Figure 4. Numerical solution for combination of first- and third-kind boundary conditions with entire-domain-filled source term (QUICK for $P_\Delta \to \infty$).

4. The Influence of Multiple Dimensions

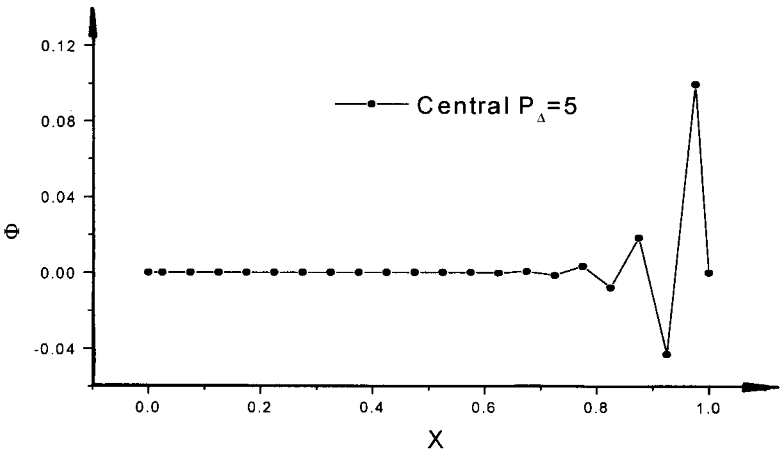
In order to investigate the effect of the space dimension, 2-D lid-driven flow in a cavity with different wall temperatures is proposed. The moving lid is at high temperature, while the other three stationary walls are at uniform but lower temperature. The thermophysical properties are assumed to be constant, hence convergent velocity fields may be obtained first, and then the temperature field computed. This is a perfect model to study the effect of the space dimension while the other four conditions remain the same as for the 1-D case. Computations were conducted for Re = 100. The local velocity components in the x and y directions are used to calculate grid Peclet numbers $P_{\Delta x}$ and $P_{\Delta y}$, respectively. It is found that for the central difference scheme no oscillation occurs until the maximum grid Peclet number is as high as about 7.1. This shows that multiple dimensions in space lead to a more robust numerical stability of the convection scheme.

5. The Effect of Nonlinearity

The discussion of the previous section is based on given velocity fields. For such cases, the governing equation is linear for the variable to be solved. The problem becomes nonlinear if the solved variable is velocity itself. By using the central difference scheme, Kong et al. [7] studied a three-dimensional lid-driven flow in a cubic cavity and found that the computational results of velocities were not



(a) With entire domain-filled source term(CDS for P_Δ=10)



(b) Without source term (CDS for P_Δ=5)

Figure 5. Numerical solutions for combination of first- and third-kind boundary conditions: (*a*) with entire-domain-filled source term (CDS for $P_\Delta = 10$); (*b*) without source term (CDS).

oscillatory even when grid Peclet number was as high as 45 in a local region, which shows the effect of both nonlinearity and multiple dimensions in space.

To this end, we may raise a very important problem for judging the numerical stability of the convective finite difference scheme: Is the grid Peclet number a unique criterion? If it is, then we believe that the critical grid Peclet number should be routine-independent. In other words, for the same situation, when we search for the critical Peclet number from its low-value case, we may increase the velocity, coarsen

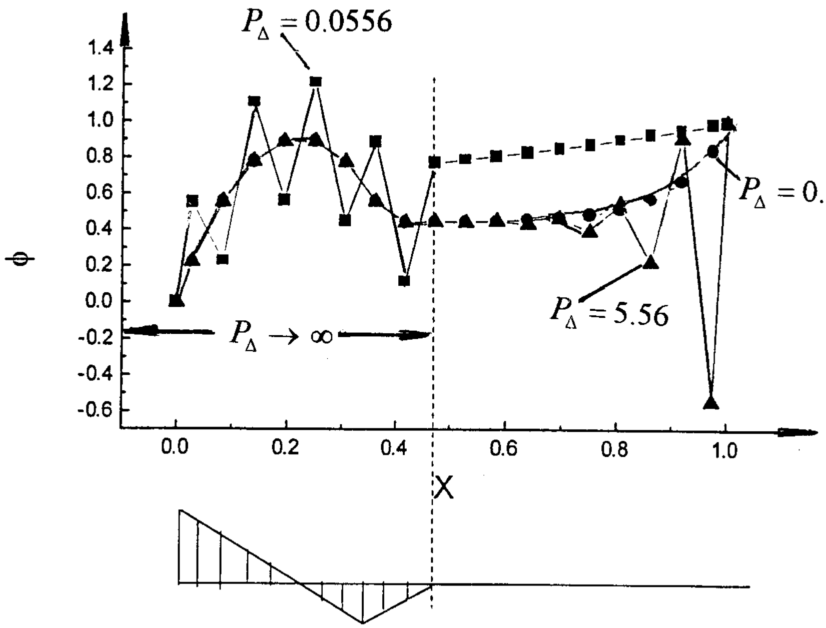


Figure 6. Effect of grid Peclet number distribution.

the grid network, decrease fluid viscosity, or we may use all the above methods simultaneously. For whatever method we use, the final value of the critical Peclet number should be the same in the numerical sense. In our numerical search of the critical Peclet number, we have found that for all one-dimensional cases we studied, the value of the critical grid Peclet number is approximately routine-independent. For multidimensional cases, however, our preliminary computations show that not all cases exhibit such character. Further research work is imperatively needed for multidimensional cases to reveal the factors which affect the numerical convective stability and the quantitative relationships among them.

BOUNDEDNESS OF CONVECTIVE FINITE-DIFFERENCE SCHEMES

Attention is now turned to the analysis of boundedness of convection schemes. First, a brief review of normalized variable formulation and the convective boundedness criterion will be given, with discussion of the relationship between stability and boundedness. Then a new region in the normalized variable diagram (NVD) will be introduced within which a bounded scheme may be defined. A new scheme defined in this new region is proposed, and three test cases are provided to demonstrate its effectiveness to avoid unphysical undershoot/overshoot behavior.

1. The Normalized Variable

In order to simplify the definition of functional relationship of high-order composite schemes, the normalized variable proposed by Leonard [13] is used in the

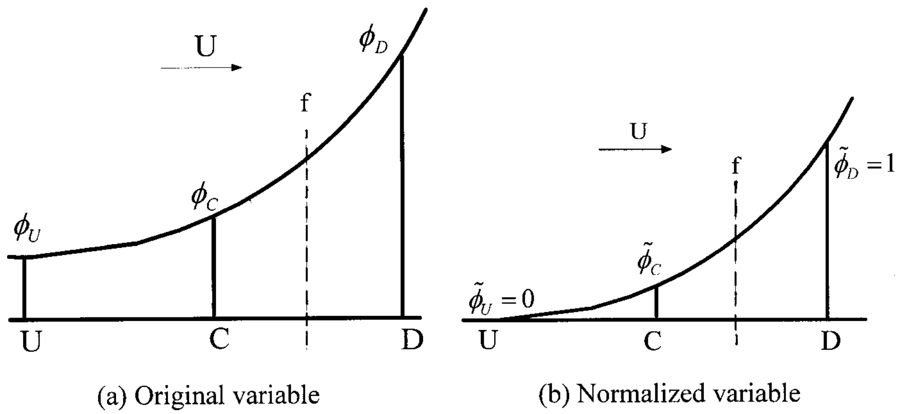


Figure 7. Stencil of interface variable interpolation: (*a*) original variable; (*b*) normalized variable.

present study. Considering three neighboring grid points as shown in Figure 7*a*, defining $\phi_U, \phi_D, \phi_C, \phi_f$ as the upstream (U), downstream (D), central (C) nodal values, and interface values (f), the definition of an upwind-biased higher-order scheme usually can be formulated as

$$\phi_f = f(\phi_U, \phi_C, \phi_D) \tag{5}$$

Now, defining a normalized variable as

$$\tilde{\phi} = \frac{\phi - \phi_U}{\phi_D - \phi_U} \tag{6}$$

we have $\tilde{\phi}_U = 0$, $\tilde{\phi}_D = 1$, and the interpolation for $\phi_f = f(\phi_U, \phi_C, \phi_D)$ is simplified to

$$\tilde{\phi} = f(\tilde{\phi}_C) \qquad \text{(Figure 7}b\text{)} \tag{7}$$

2. Stability Judgment via NVD

Taking $\tilde{\phi}_C$ and $\tilde{\phi}_f$ as the abscissa and ordinate, respectively, we may outline many schemes in this coordinate system (often called a normalized variable diagram, NVD) by a single straight line. In Figure 8*a*, six such schemes are presented, where SUS and TUS represent the second-order upwind and third-order upwind schemes, respectively. For simplicity of presentation, we shall call such a line the characteristic line of the scheme. In Table 1, their definitions are provided in both usual and normalized variables. It is interesting to note that the critical Peclet number of a scheme determined from the one-dimensional analysis may be obtained from its characteristic line in the NVD. Actually, the intersection of the characteristic line and the ordinate of the NVD equals the coefficient of the downstream point in the conventional definition of a scheme (Table 2); and the value of this coefficient is equal to the reciprocal of the critical Peclet number of the scheme.

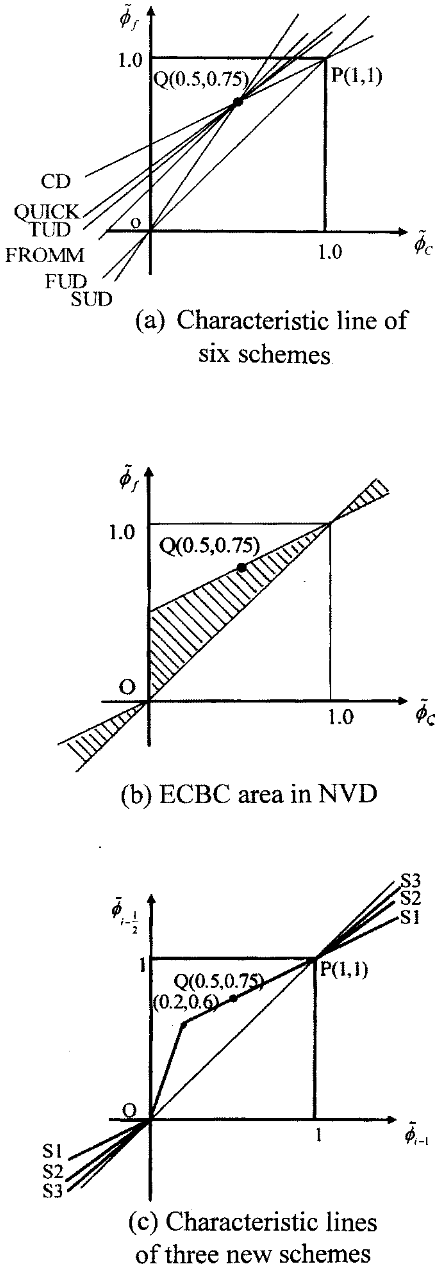


Figure 8. Representation of different schemes in NVD: (*a*) characteristic lines of six schemes; (*b*) ECBC area in NVD; (*c*) characteristic lines of three new schemes.

Thus we may come to the conclusion that for a convective scheme to be unconditionally stable, its characteristic line in the NVD must go though the coordinate original point (0, 0).

Table 1. Definitions of six schemes in conventional and normalized forms

No.	Scheme name	Conventional definition	Normalized definition
1	FUS	$\phi_f = \phi_C$	$\tilde{\phi}_f = \tilde{\phi}_C$
2	CDS	$\phi_f = \frac{1}{2}(\phi_C + \phi_D)$	$\tilde{\phi}_f = \frac{1}{2}(\tilde{\phi}_C + 1) = 0.75 + 0.5(\tilde{\phi}_C - 0.5)$
3	SUS	$\phi_f = \frac{3}{2}\phi_C - \frac{1}{2}\phi_U$	$\tilde{\phi}_f = \frac{3}{2}\tilde{\phi}_C = 0.75 + 1.5(\tilde{\phi}_C - 0.5)$
4	QUICK	$\phi_f = \frac{1}{8}(3\phi_D + 6\phi_C - \phi_U)$	$\tilde{\phi}_f = \frac{1}{8}(3 + 6\tilde{\phi}_C) = 0.75 + 0.75(\tilde{\phi}_C - 0.5)$
5	Fromm [25]	$\phi_f = \frac{1}{4}(\phi_D + 4\phi_C - \phi_U)$	$\tilde{\phi}_f = \frac{1}{4}(1 + 4\tilde{\phi}_C) = 0.75 + (\tilde{\phi}_C - 0.5)$
6	TUS	$\phi_f = \frac{1}{6}(2\phi_D + 5\phi_C - \phi_U)$	$\tilde{\phi}_f = \frac{1}{6}(2 + 5\tilde{\phi}_C) = 0.75 + \frac{5}{6}(\tilde{\phi}_C - 0.5)$

Table 2. Relationship between $P_{\Delta cr}$ and coefficients of ϕ_D

Scheme	Coefficient of ϕ_D	Intersection	$P_{\Delta cr}$
CD	$\frac{1}{2}$	0.5	2
QUICK	$\frac{3}{8}$	0.375	$\frac{8}{3}$
TUD	$\frac{1}{3}$	0.333	3
Fromm	$\frac{1}{4}$	0.25	4
SUS	0	0	∞
FUS	0	0	∞

3. The Convective Boundedness Criterion (CBC)

Gaskell and Lau proposed the convective boundedness criterion based on normalized variable analysis, which states the conditions for boundedness as follows:

$$\tilde{\phi}_f = f(\tilde{\phi}_C) = \tilde{\phi}_C \qquad \text{for } \tilde{\phi}_C \le 0 \tag{8a}$$

$$\tilde{\phi}_f = f(\tilde{\phi}_C) = \tilde{\phi}_C \qquad \text{for } \tilde{\phi}_C \ge 1 \tag{8b}$$

$$\tilde{\phi}_C \le \tilde{\phi}_f \le 1 \qquad \text{for } 0 < \tilde{\phi}_C < 1 \tag{8c}$$

In Figure 1, the shaded region and the diagonal, which goes through the points (0, 0) and (1, 1) in the NVD, represent the CBC. This means that if the characteristic line of a convection scheme is located within this shaded area for $\tilde{\phi}_c \in [0, 1]$ and coincides with the diagonal for $\tilde{\phi}_c$ outside [0, 1], the scheme possesses boundedness. As mentioned above, many authors, including Gaskell and Lau, consider that the above conditions are both sufficient and necessary for convective boundedness. And all the existing high-resolution schemes, including the newly proposed scheme WACEB [26], are defined within the region prescribed by Eq. (8).

4. The Extended Convective Boundedness Criterion (ECBC)

Our numerical experiments show that the CBC proposed by Gaskell and Lau is only a sufficient condition. In other words, there may be another region(s) in the NVD within which the characteristic lines of bounded schemes may be located. The present authors have found that schemes satisfying the following constraints are also bounded:

$$\tilde{\phi}_C \le \tilde{\phi}_f \le \frac{\tilde{\phi}_C}{2} \qquad \text{for } \tilde{\phi}_C \le 0 \tag{9a}$$

$$\tilde{\phi}_C \le \tilde{\phi}_f \le \frac{\tilde{\phi}_C + 1}{2} \qquad \text{for } 0 < \tilde{\phi}_C < 1 \tag{9b}$$

$$\frac{\tilde{\phi}_C + 1}{2} \le \tilde{\phi}_f \le \tilde{\phi}_C \qquad \text{for } \tilde{\phi}_C \ge 1 \tag{9c}$$

This constraint is called the extended convective boundedness criterion (ECBC). The shaded area in Figure 8*b* represents this bounded criterion. In what follows, normalized variable analysis will be used to elucidate the ECBC. As usual, the case of one-dimensional flow with constant velocity u and diffusion coefficient Γ is assumed which is formulated by Eq. (4). The normalized integral form of Eq. (4) over the control volume (Figure 9) can be written as

$$\tilde{\phi}_f - \tilde{\phi}_{f'} = \frac{\phi_f - \phi_{f'}}{\phi_D - \phi_U} = \tilde{S}^* \tag{10}$$

where the effective normalized source term $\tilde{S}^*$ is composed of diffusion and physical source terms and takes the following form:

$$\tilde{S}^* = \frac{[\Gamma(d\phi/dx)]_f - [\Gamma(d\phi/dx)]_{f'} + \int_{f'}^{f} S(x)\, dx}{\rho\, u(\phi_D - \phi_U)} \tag{11}$$

As indicated by Gaskell and Lau [12], the following constraints can ensure computational boundedness:

$$1 < \tilde{\phi}_f \le \tilde{\phi}_C, 0 \le \tilde{\phi}_{f'} < \tilde{\phi}_f \qquad \text{for } \tilde{S}^* > 0, \tilde{\phi}_C > 1 \tag{12a}$$

$$0 \le \tilde{\phi}_{f'} \le \tilde{\phi}_C < \tilde{\phi}_f \le 1 \qquad \text{for } \tilde{S}^* \ge 0, 0 \le \tilde{\phi}_C \le 1 \tag{12b}$$

$$\tilde{\phi}_C \le \tilde{\phi}_f < \tilde{\phi}_{f'} < 0 \qquad \text{for } \tilde{S}^* < 0, \tilde{\phi}_C < 0 \tag{12c}$$

It can be shown that the ECBS meets the above constraints.

First, it can be seen from Figure 9 that cell face values $\tilde{\phi}_f$ defined in Eq. (12) are somewhat between those obtained from a first-order-upwind scheme and a central difference scheme, i.e., the values of ϕ_f and $\phi_{f'}$ defined in Eq. (12) satisfy the following condition:

$$\phi_f \in \{\min[\phi_C, (\phi_C + \phi_D)/2], \max[\phi_C, (\phi_C + \phi_D)/2]\} \tag{13a}$$

$$\phi_{f'} \in \{\min[\phi_U, (\phi_U + \phi_C)/2], \max[\phi_U, (\phi_U + \phi_C)/2]\} \tag{13b}$$

Equation (13) will be recast into normalized form for the three variation ranges of $\tilde{\phi}_C$.

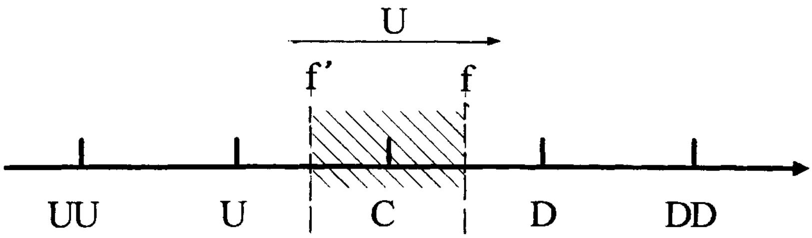


Figure 9. Control volume of one-dimensional grid system.

1. For $\tilde{S}^* > 0$, $\tilde{\phi}_C > 1$, Eqs. (13a) and (13b) lead to the following two inequalities, respectively:

$$\tilde{\phi}_f \in [\tilde{\phi}_C, (\tilde{\phi}_C + 1)/2] \tag{14a}$$

$$\tilde{\phi}_{f'} \in [0, \tilde{\phi}_C/2] \tag{14b}$$

Thus we have

$$1 < \tilde{\phi}_f \leq \tilde{\phi}_C \qquad 0 \leq \tilde{\phi}_{f'} < \tilde{\phi}_f \tag{a}$$

2. For $\tilde{S}^* \geq 0$, $0 \leq \tilde{\phi}_C \leq 1$, the normalized form of Eqs. (13a) and (13b) are the same as those of Eqs. (14a) and (14b), which now can be combined into

$$0 \leq \tilde{\phi}_f \leq \tilde{\phi}_C < \tilde{\phi}_f \leq 1 \tag{b}$$

3. For $\tilde{S}^* < 0$, $\tilde{\phi}_C < 0$, Eq. (13a) becomes

$$\tilde{\phi}_f \in [\tilde{\phi}_C, (\tilde{\phi}_C + 1)/2] \tag{c}$$

From the specified condition, Eq. (9a), we have

$$\tilde{\phi}_f \in [\tilde{\phi}_C, \tilde{\phi}_C/2] \tag{d}$$

In addition, Eq. (13b) becomes

$$\tilde{\phi}_{f'} \in [\tilde{\phi}_C/2, 0] \tag{e}$$

Combining Eqs. (d) and (e) we obtain

$$\tilde{\phi}_C \leq \tilde{\phi}_f \leq \tilde{\phi}_{f'} < 0 \tag{f}$$

From the above discussion, we can see that the ECBC is a sufficient condition for convective boundedness.

5. SBECBC

In the present work three new schemes are proposed in the region of the ECBC. Since the major difference between the CBC and the ECBC is in the regions of $\tilde{\phi}_C \leq 0$ and $\tilde{\phi}_C \geq 1.0$, the definitions of the three new schemes are all the same in the region of $\tilde{\phi} \in [0, 1.0]$, with different characteristic lines in the region outside $\tilde{\phi} \in [0, 1.0]$. The three new schemes are formulated as follows:

$$\text{SBECBC1} \quad \tilde{\phi}_f = \tilde{\phi}_C/2 \quad \text{for } \tilde{\phi}_C \le 0 \tag{15a}$$
$$\tilde{\phi}_f = 3\tilde{\phi}_C \quad \text{for } 0 < \tilde{\phi}_C < 0.2 \tag{15b}$$
$$\tilde{\phi}_f = (\tilde{\phi}_C + 1)/2 \quad \text{for } \tilde{\phi}_C \ge 0.2 \tag{15c}$$
$$\text{SBECBC2} \quad \tilde{\phi}_f = 3\tilde{\phi}_C/4 \quad \text{for } \tilde{\phi}_C \le 0 \tag{16a}$$
$$\tilde{\phi}_f = 3\tilde{\phi}_C \quad \text{for } 0 < \tilde{\phi}_C < 0.2 \tag{16b}$$
$$\tilde{\phi}_f = (\tilde{\phi}_C + 1)/2 \quad \text{for } 0 < \tilde{\phi}_C \le 1 \tag{16c}$$
$$\tilde{\phi}_f = (3\tilde{\phi}_C + 1)/4 \quad \text{for } \tilde{\phi}_C > 1 \tag{16d}$$
$$\text{SBECBC3} \quad \tilde{\phi}_f = 7\tilde{\phi}_C/8 \quad \text{for } \tilde{\phi}_C \le 0 \tag{17a}$$
$$\tilde{\phi}_f = 3\tilde{\phi}_C \quad \text{for } 0 < \tilde{\phi}_C < 0.2 \tag{17b}$$
$$\tilde{\phi}_f = (\tilde{\phi}_C + 1)/2 \quad \text{for } 0 < \tilde{\phi}_C \le 1 \tag{17c}$$
$$\tilde{\phi}_f = (7\tilde{\phi}_C + 1)/8 \quad \text{for } \tilde{\phi}_C > 1 \tag{17d}$$

These schemes are based on the extended convection boundedness criterion, hence are called SBECBC with different digits as suffixes to indicate different versions. The three schemes are illustrated in Figure 8*c*, where S1, S2, and S3 represent SBECBC1, SBECBC2, and SBECBC3, respectively.

6. Test Examples

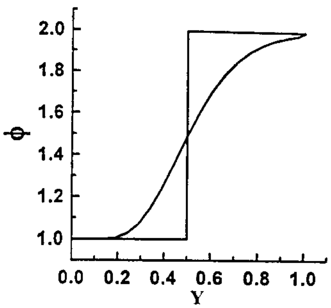
We adopted SBECBCs to compute the transport of a scalar field with discontinuities in its gradient by pure convection. The problems of purely convective transport of a scalar field with discontinuities are widely used to test high-order composite schemes for boundedness. The computational results are considered converged when the residual error given by Eq. (18) becomes less than 0.05%:

$$\text{Res} = \sum \left| A_P \phi_P - \left(\sum_{\text{nb}} A_{\text{nb}} \phi_{\text{nb}} + S_P + S_A \right) \right| \tag{18}$$

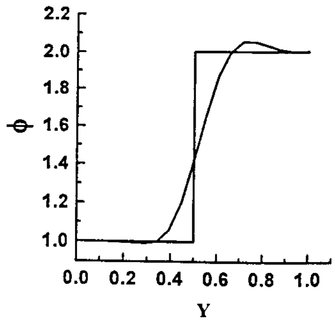
The first test problem is convection of a step profile in an oblique velocity field. The given velocity fields of the test problem are as follows:

$$x = 0 \quad 0 \le y \le 0.5(1 - \tan 35^\circ) \quad \phi = 1$$
$$x = 0 \quad 0.5(1 - \tan 35^\circ) < y \le 1 \quad \phi = 2$$
$$0 \le x \le 1 \quad y = 0,\ \phi = 1$$
$$u = \cos 35^\circ \quad v = \sin 35^\circ$$

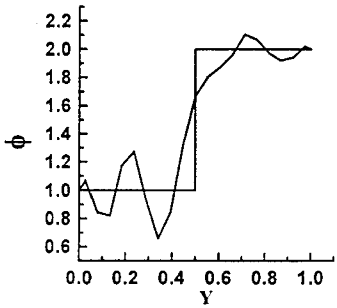
A comparison of the numerical solutions at the vertical central plan of the solution domain computed by 12 different schemes with a 21×21 uniform mesh is presented in Figure 10. It can been seen that the solution from the FUS is extremely diffusive. The numerical results of the second-order upwind difference scheme (SUS), CD, and QUICK produce results with strong oscillations and overshoot/undershoot. On the



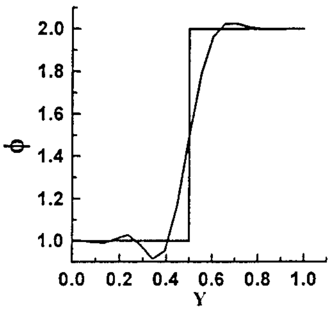
(a) Solution of FUS



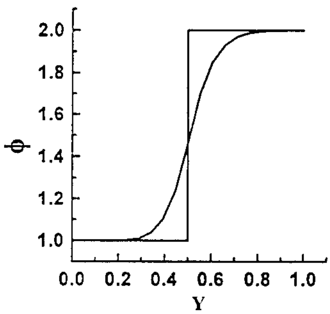
(b) Solution of SUS



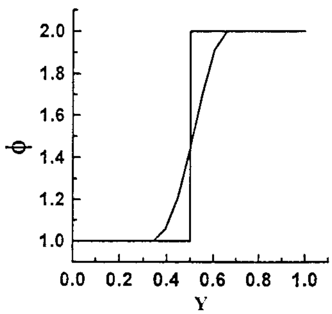
(c) Solution of CDS



(d) Solution of QUICK



(e) Solution of MINMOD



(f)Solution of OSHER

Figure 10(a)–(f). *Continued*

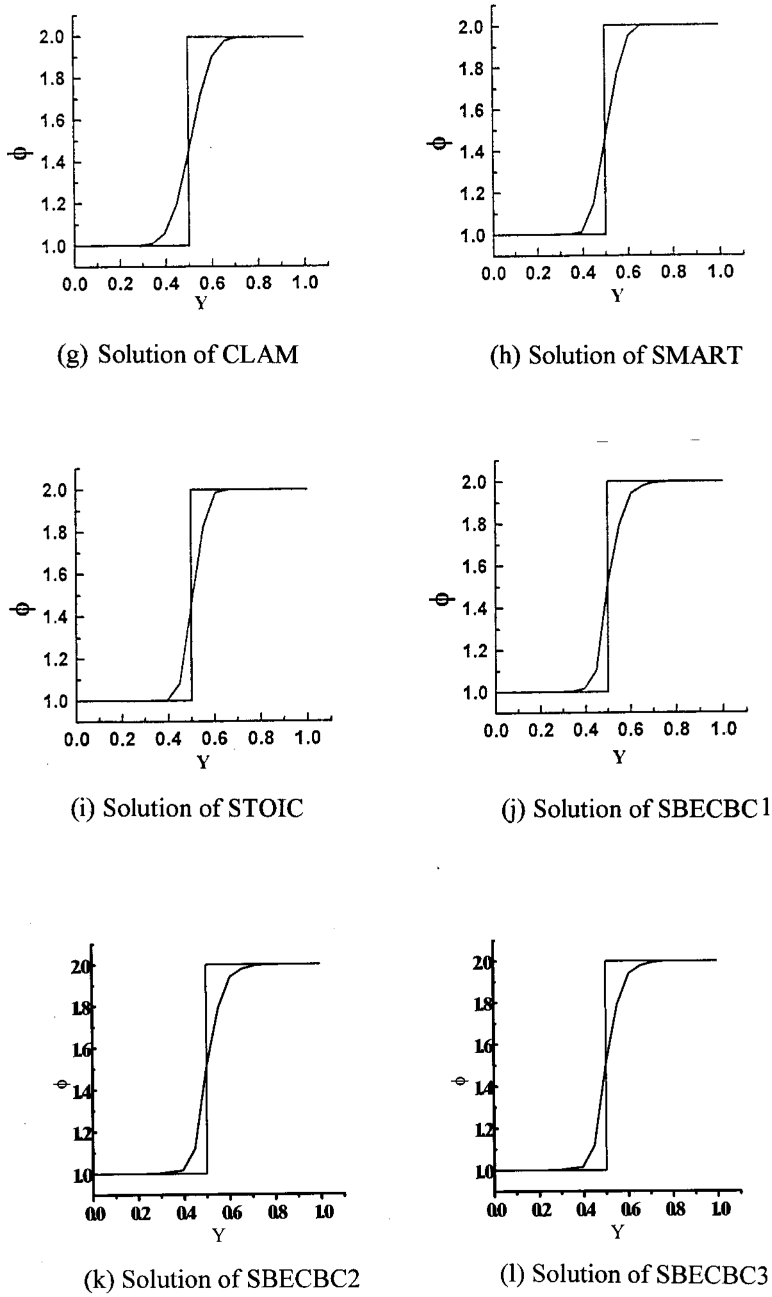


Figure 10. Comparison of velocity profiles at the vertical central plane from different schemes: (*a*) FUS; (*b*) SUS; (*c*) CDS; (*d*) QUICK; (*e*) MINMOD; (*f*) OSHER; (*g*) CLAM; (*h*) SMART; (*i*) STOIC; (*j*) SBECBC1; (*k*) SBECBC2; (*l*) SBECBC3.

Table 3. Comparison of average error of different schemes

Scheme	CD	SUD	QUICK	FROMM	MINMOD	SMART
Error × 100	10.200	4.1570	4.0661	3.8378	4.7446	2.9223
Scheme	STOIC	SECBC1	SECBC2	SECBC3	OSHER	MUSCL
Error × 100	2.2178	2.8648	2.8684	2.8684	3.6082	3.1788

other hand, all high-order composite schemes, namely, CLAM, OSHER, MINMOD, SMART, STOIC, and SBECBC1, 2, 3, give physically reasonable results. To qualify the numerical accuracy of different schemes, an average error is defined as follows:

$$E_{\mathrm{av}} = \frac{1}{N}\sum_{n}^{N}\left|\frac{\phi_{n,\mathrm{exact}} - \phi_{n,\mathrm{numerical}}}{\phi_{n,\mathrm{exact}}}\right| \tag{19}$$

The average errors of the numerical results of different schemes are listed in Table 3. It can be seen that the STOIC scheme gives the most accurate simulation, followed by the SBECBCs family and SMART.

Our second test problem is advection of a square scalar field in a given velocity field skewed at an angle of 45° with respect to the meshes. The 2-D domain is shown in Figure 11*a*, and a 3-D perspective view of the initial field is presented in Figure 11*b*. The maximum and minimum values of the field are 10 and 0.0, respectively. Computations were conducted using three new schemes. Since the results are essentially the same, only the results of SBECBC1 are presented. Figures 11*c*–11*f* depict the advection process predicted by SBECBC1. It can be seen clearly that SBECBC1 gives oscillation-free results.

The last example is the two-dimensional lid-driven cavity flow. This is a convection-diffusion problem. The convection term is discretized by SBECBC1, 2, 3 and the diffusion term by central difference. The computational results are compared with the benchmark solution [27]. Since the curve representations of the three solutions of SBECBC1, 2 and 3 can hardly be distinguished, only the results of SBECBC1 are compared with the benchmark solution. The velocity distributions at two mid-cross sections are presented at Figure 12. The very good agreement between the numerical results and the benchmark solution can be clearly observed.

CONCLUSIONS

The main findings of the present article can be summarized as follows.

1. Existing analysis methods for the stability of a discretized convective term are based on five assumptions. Thus, obtained critical grid Peclet number is the most severe requirement for convective stability.
2. When a conditionally stable scheme, such as QUICK or central differencing is adopted to discretize a practical problem, oscillation-free solution may be obtained under much greater grid Peclet than that predicted by the existing

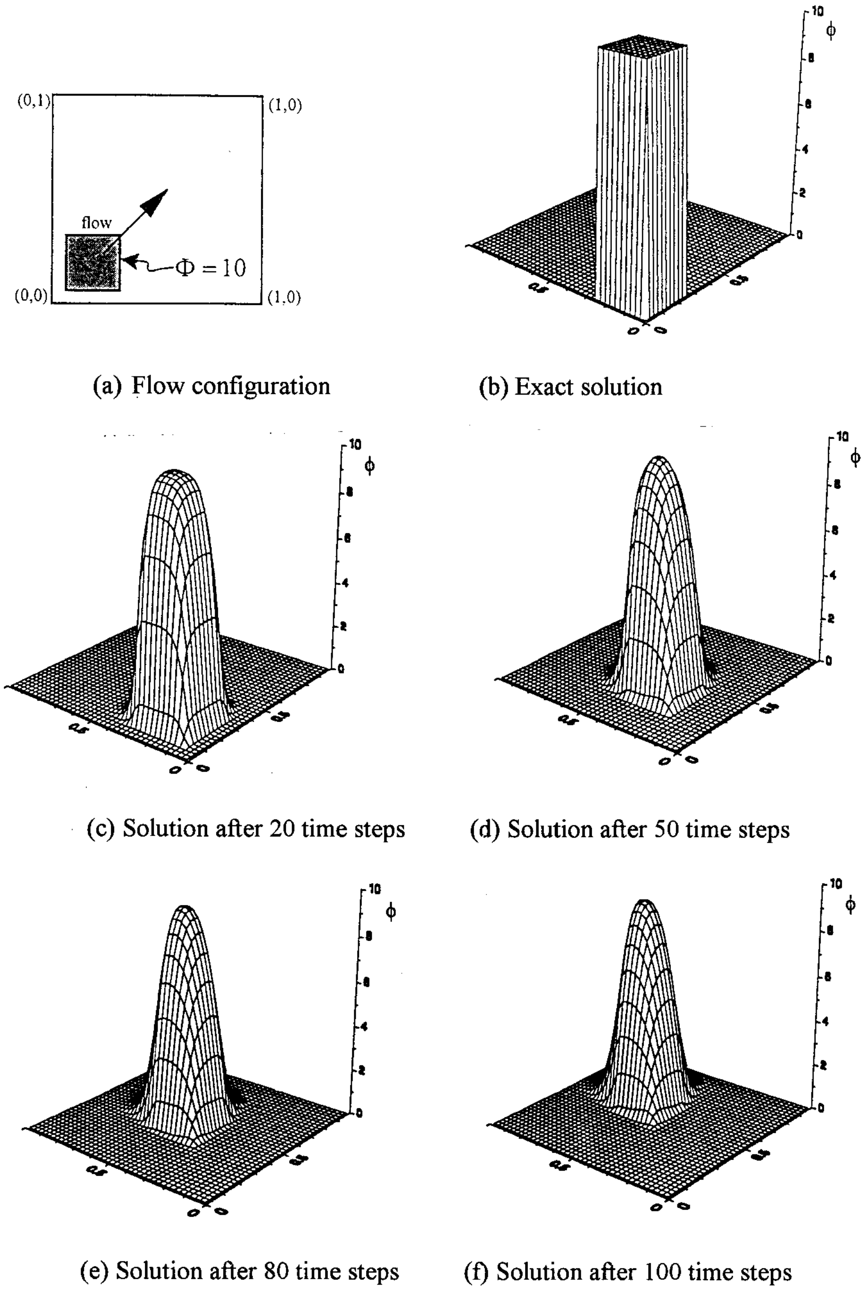
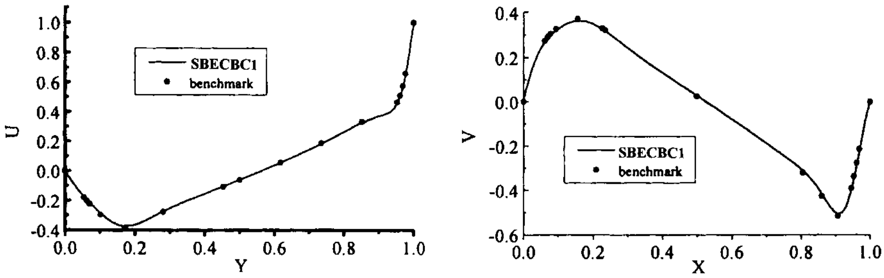


Figure 11. Transport of a square scalar field in a given velocity field predicted by SBECBC1: (*a*) flow configuration; (*b*) initial filed; (*c*) numerical solution after 20 time steps; (*d*) numerical solutions after 50 time steps; (*e*) numerical solutions after 80 time steps; (*f*) numerical solution after 100 time steps.



(a) U-velocity (b) V-velocity

Figure 12. Velocity distributions at mid-planes for lid-driven cavity flow.

analysis methods. Any deviation from the five assumptions of the existing analyses may attribute, more or less, to enhance convective stability.

3. For a convective scheme to be absolutely stable, its characteristic line in the NVD must goes through the original point. The reciprocal of the intersection of the characteristic line with the ordinate is equal to the critical Peclet number from the one-dimensional analysis.
4. The CBC defined by Gaskell and Lau is only a sufficient criterion for boundedness. The convective bounded region in the NVD can be extended, and a new region has been discovered.
5. Three new high-order bounded schemes called SBECBC1, 2, and 3 are proposed. Numerical computations with the SBECBCs are performed for three test problems containing discontinuities in gradient, and no overshoot/undershoot is found. The new schemes are compared with six other high-order composite schemes for a pure convection problem of scalar profile with steep gradient, and it is found that their numerical accuracy is slightly better than that of SMART.
6. The convection term in the 2-D Navier-Stokes equation was discretized by SBECBCs and the resulting discretized equations were used to solve the lid-driven cavity flow by the SIMPLER algorithm. The numerical results agree well with the benchmark solution, indicating the feasibility of the proposed schemes in the simulation of both advection and convection-diffusion problems.

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