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Refinement of the convective boundedness criterion of Gaskell and Lau

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Abstract *Based on the normalized variable diagram, the weakness of the Gaskell and Lau's convective boundedness criterion (GL-CBC) is revealed by numerical example. By careful consideration of the smoothness of the normalized variable variation pattern, more rigorous constraints on the interface value interpolation are found. A new CBC is thus proposed, whose feasibility and correctness are demonstrated by the inspection of ten existing bounded schemes and a numerical example.*

Nomenclature

f	= cell face	*Subscripts*	
ϕ	= general dependent variable	$i-1$	= central grid point
Γ	= diffusion coefficient	i	= downstream grid point
s	= source term in the discretized equation	$i-2$	= upstream grid point
u	= velocity in the X direction	$i-3/2, i-1/2$	= refer to control volume face

1. Introduction

Successful simulation of convection-diffusion problems 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. For the diffusion term, the second-order finite difference scheme, central difference, works very well and is almost unanimously adopted in most engineering computations. While for convection term, a variety of choices can be made. It is well known that stability, boundedness and accuracy are the most important properties of modeling schemes for convection term. In developing a computational program for fluid flow and heat transfer problems, it is desired to adopt a modeling scheme for convection, possessing high accuracy,

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high stability and boundedness characteristics with reasonable computational effort. But in practice no scheme proposed so far has been proved to possess such virtues simultaneously. The difficulty in devising a satisfactory scheme lies in the conflicting requirements of accuracy on one hand, stability and boundedness on the other. Generally, accuracy is regarded as the order of modeling scheme truncation error. Proverbially, high-order (second-order or the higher) 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 scheme (FUS) often suffer severe inaccuracies due to the so-called false diffusion resulted from the low-order truncation error. Physically speaking, when the convection term is discretized by a bounded scheme, the resulting numerical solution will never overpass the maximum or minimum values inherently determined by the physical process itself. For example, the concentration of a component of a mixture can be varied only 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), it is said that the convection scheme does not possess the boundedness. Since the overshoot or undershoot always occur at position where a steep gradient of dependent variable exists, boundedness of a scheme may be defined as to predict no unphysical oscillations in regions of steep gradients (Song *et al.*, 2000). Obviously, boundedness is of immense importance to keep numerical results physically reasonable.

Gaskell and Lau (1988) proposed a criterion for a convection scheme to possess the boundedness character and named the criterion as convective boundedness criterion (CBC). In addition, they also delineated a corresponding region in the normalized variable diagram (NVD) shown in Figure 1 by the shadowed 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. Noticeably, in CFD, there is another constraint, called total variation diminishing (TVD), and is often used for construction of a modeling scheme for convection. The relationship between CBC and TVD was revealed by Lin and Lin (1997). It turns out that the constraint of TVD is more restrictive than Gaskell/Lau's CBC, and can be represented by the shaded area in NVD shown in Figure 2. Usually, the TVD requirement is applied to the compressible flow in which the convected variable may experience sharp changes in gradients or discontinuity at position where shock wave exists. The satisfaction of TVD can guarantee that no unrealistic oscillatory results will occur in the computation of compressible flow. The CBC requirement proposed in the work of Gaskell and Lau (1988) is mainly applied to the incompressible flow, and this restriction will be retained in this paper. However, since schemes satisfying the constraint of TVD are always bounded (but not vice versa), therefore they will be referred to as bounded schemes and may be compared with other schemes that only satisfy the CBC condition. Considerable efforts have been made in recent years

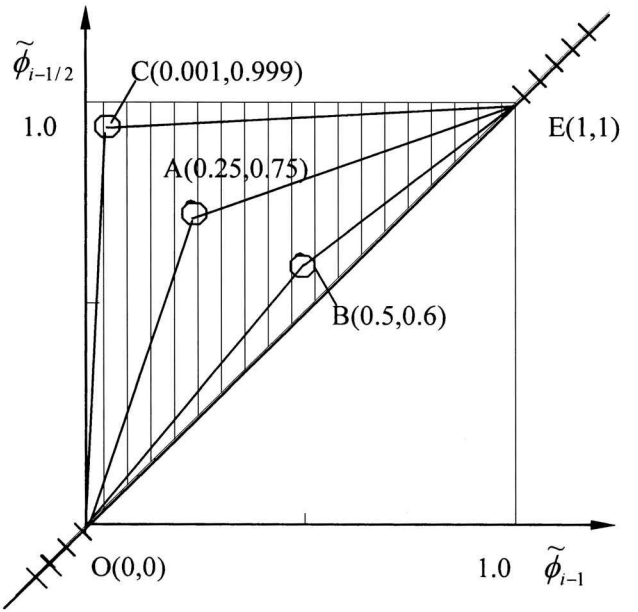


Figure 1.
NVD and the region of CBC

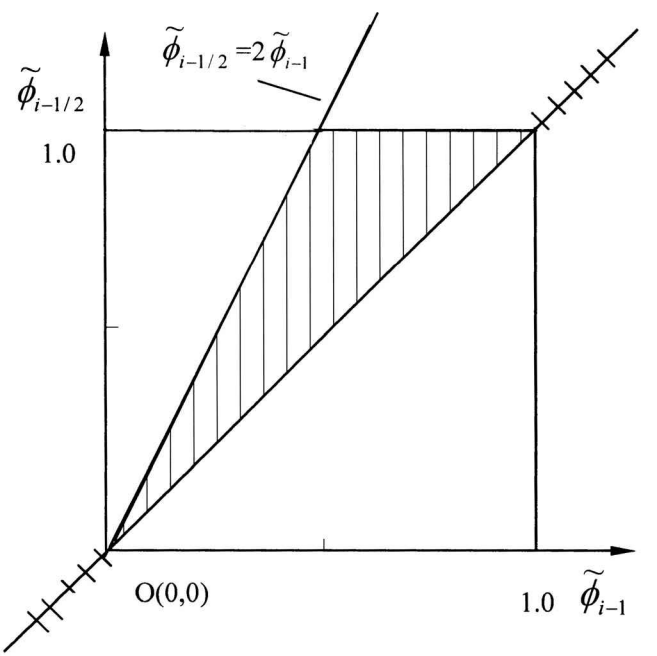


Figure 2.
Representation of TVD constraint in NVD

to develop what is called as high-resolution composite schemes to overcome the unphysical overshoot/undershoot behavior of some high-order schemes such as QUICK (Leonard, 1979). A number of high-resolution composite schemes were proposed for the calculation of viscous fluid flow with finite volume methods. The schemes are, for example, MUSCL (Leer, 1977), CLAM (Zhu, 1991), OSHER (Chakravarthy and Osher, 1983), MINMOD (Zhu and Rodi, 1991), SMART (Gaskell and Lau, 1988), STOIC (Darvish, 1993), COPLA (Choi *et al.*, 1995), EULER (Leonard, 1983), and WACEB (Song *et al.*, 2000), which all satisfy the CBC.

The CBC and the restricted region in the NVD have long been accepted as both the sufficient and necessary condition for a scheme possessing boundedness (Choi *et al.*, 1995; Darvish, 1993; Gaskell and Lau, 1988). Very recently, Tao (2000) and Yu *et al.* (2001) indicated that the CBC proposed by Gaskell and Lau (hereafter GL-CBC for simplicity) is only a sufficient condition, and they proposed another CBC, named as extended CBC (ECBC). Two new schemes were designed according to the ECBC, and their numerical experiments show that the two new schemes work well, both possess the convective boundedness and high accuracy.

In this paper, further improvements will be made to the GL-CBC based on the smoothness considerations of the variable profile, and a new region for a scheme to possess the boundedness and high accuracy in the NVD will be delineated. Any scheme whose characteristic line is located in the new region possess both boundedness and high accuracy (i.e. at least with second-order of truncation error). It turns out that the CBC regions where $\tilde{\phi}_{i-1} < 0$ or $\tilde{\phi}_{i-1} > 1$ proposed in this paper coincide with that of ECBC. In the following, the weakness of the GL-CBC will first be illustrated, and the necessity and the sufficiency of the GL-CBC will be discussed further. Then the detailed discussion will be presented on the desired interface interpolation in the different regions between $\tilde{\phi}_{i-1} = 0$ and $\tilde{\phi}_{i-1} = 1$, so that the resulting profile of the variable studied will have better smoothness. A new CBC region will be delineated in the NVD according to the discussion. The characteristic lines of ten existing high resolution schemes will be checked to see if they are all located in the new region, and it turns out to be the case. Finally, numerical examples will be presented to show the feasibility of the new CBC.

2. Normalized variable and the weakness of GL-CBC

In order to simplify the definition of functional relationship of high-order composite schemes, the normalized variable proposed by Leonard (1979) is used in the present study. Considering three neighboring grid points shown in Figure 3(a), defining $\tilde{\phi}_{i-2}, \tilde{\phi}_i, \tilde{\phi}_{i-1}, \tilde{\phi}_{i-1/2}$ as the upstream ($i-2$), downstream (i), central ($i-1$) nodal values and interface values ($i-1/2$), the definition of an upwind-biased higher-order scheme can be formulated as

$$\phi_{i-1/2} = f(\phi_{i-2}, \phi_{i-1}, \phi_i) \tag{1}$$

Now defining a normalized variable as:

$$\tilde{\phi} = \frac{\phi - \phi_{i-2}}{\phi_i - \phi_{i-2}} \tag{2}$$

Then we have $\tilde{\phi}_{i-2} = 0$, $\tilde{\phi}_i = 1$, and the interpolation for $\tilde{\phi}_{i-1/2} = f(\tilde{\phi}_{i-2}, \tilde{\phi}_{i-1}, \tilde{\phi}_i)$ is simplified to

$$\tilde{\phi}_{i-1/2} = f(\tilde{\phi}_{i-1}) \tag{3}$$

The stencil of the normalized variable is shown in Figure 3(b). It should be noted that for the convenience of comparison with Gaskell and Lau (1988), the numbering system of Gaskell and Lau (1988) is adopted here.

In order to establish restrictions on the interface interpolation rules, the one-dimensional diffusion-convection equation for fluid with a source term is used:

$$\begin{gathered} \frac{\mathrm{d}(\rho u \phi)}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x}\right) + S(x) \\ x = 0,\ \phi = \phi_0;\ x = L,\ \phi = \phi_L \end{gathered} \tag{4}$$

where ϕ is a general dependent scalar variable, Γ is a nominal diffusion coefficient.

For the case of constant velocity u and Γ, the normalized integral of equation (4), over this control volume can be written as

$$\tilde{\phi}_{i-1/2} - \tilde{\phi}_{i-3/2} = \frac{\phi_{i-1/2} - \phi_{i-3/2}}{\phi_i - \phi_{i-2}} = \tilde{S}^* \tag{5}$$

where $\tilde{S}^*$ is the net effective normalized source term, comprised of diffusion and physical source term:

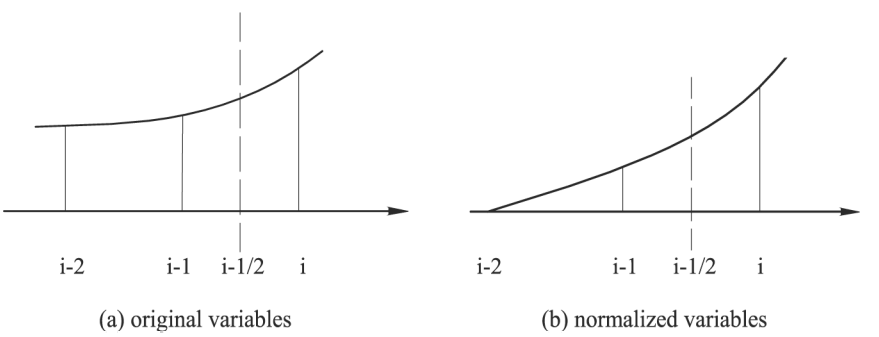


Figure 3. Stencil of interface variable interpolation

$$\tilde{S}^* = \frac{\left(\Gamma \frac{\mathrm{d}\phi}{\mathrm{d}x}\right)_{i-3/2}^{i-1/2} + \int_{i-3/2}^{i-1/2} S(x)\,\mathrm{d}x}{\rho u\,(\phi_i - \phi_{i-2})} \tag{6}$$

Figure 4 shows all possible variations of $\widehat{\phi}$ across the three successive grid points in physical space for different combination scenarios of $\tilde{S}^*$ and $\tilde{\phi}_{i-1}$. From Figure 4 constraints that ensure computed boundedness of $\widehat{\phi}_{i-1/2}$ can be given as follows (Gaskell and Lau, 1988):

$$\begin{aligned}
&0 \le \tilde{\phi}_{i-3/2} \le \tilde{\phi}_{i-1} < \tilde{\phi}_{i-1/2} \le 1 \quad \text{for} \quad \tilde{S}^* \ge 0,\ 0 \le \tilde{\phi}_{i-1} \le 1 \\
&1 < \tilde{\phi}_{i-1/2} \le \tilde{\phi}_{i-1}, \quad 0 \le \tilde{\phi}_{i-3/2} < \tilde{\phi}_{i-1/2} \quad \text{for} \quad \tilde{S}^* > 0, \tilde{\phi}_{i-1} > 1 \\
&\tilde{\phi}_{i-1} \le \tilde{\phi}_{i-1/2} \le \tilde{\phi}_{i-3/2} < 0 \quad \text{for} \quad \tilde{S}^* < 0, \tilde{\phi}_{i-1} < 0
\end{aligned} \tag{7}$$

According to equation (7), Gaskell and Lau proposed that a continuous function or a piecewise continuous function $\widehat{\phi}_{i-1/2} = f(\tilde{\phi}_{i-1})$ will possess the boundedness if the following conditions are satisfied:

$$\begin{aligned}
&\tilde{\phi}_{i-1/2} = f(\tilde{\phi}_{i-1}) = \tilde{\phi}_{i-1} \quad \text{for} \quad \tilde{\phi}_{i-1} \le 0 \\
&\tilde{\phi}_{i-1/2} = f(\tilde{\phi}_{i-1}) = \tilde{\phi}_{i-1} \quad \text{for} \quad \tilde{\phi}_{i-1} \ge 1 \\
&\tilde{\phi}_{i-1} \le f(\tilde{\phi}_{i-1}) \le 1 \quad \text{for} \quad 0 < \tilde{\phi}_{i-1} < 1
\end{aligned} \tag{8}$$

The GL-CBC region in the NVD is shown in Figure 1 by the shaded area. As indicated earlier, the shaded area and the two diagonals outside the region of $\tilde{\phi}_{i-1} \in [0, 1.0]$, can guarantee that the scheme possesses boundedness. However, because the GL-CBC did not pay attention to the profile smoothness within $\tilde{\phi}_{i-1} \in [0, 1.0]$, some schemes which satisfy the GL-CBC condition may have odd variable profile and this ultimately leads to the deterioration of the solution accuracy. To illustrate, take point A (0.25, 0.75) in the NVD as an example. Suppose that a new scheme is designed whose characteristic line within the region of $\tilde{\phi}_{i-1} \in [0, 1.0]$ composes of two pieces of straight lines EA and AO as shown in Figure 1. Now we construct a figure in which the variation pattern of $\tilde{\phi}$ in one-dimensional space is presented. With the given values of $\tilde{\phi}_{i-1}$ and $\tilde{\phi}_{i-1/2}$, we get the curve shown in Figure 5(a). Obviously, this variation pattern of $\tilde{\phi}$ is unrealistic. Similar result will be obtained if we take the point B (0.5, 0.6) (Figure 1) as the corner point of a characteristic line, the resulting variation pattern of $\tilde{\phi}_{i-1}$ is shown in Figure 5(b). The situation is even worse if we take the point C (0.001, 0.999) in the NVD. In this case, an unphysical variation with over and undershoots results as shown in Figure 5(c).

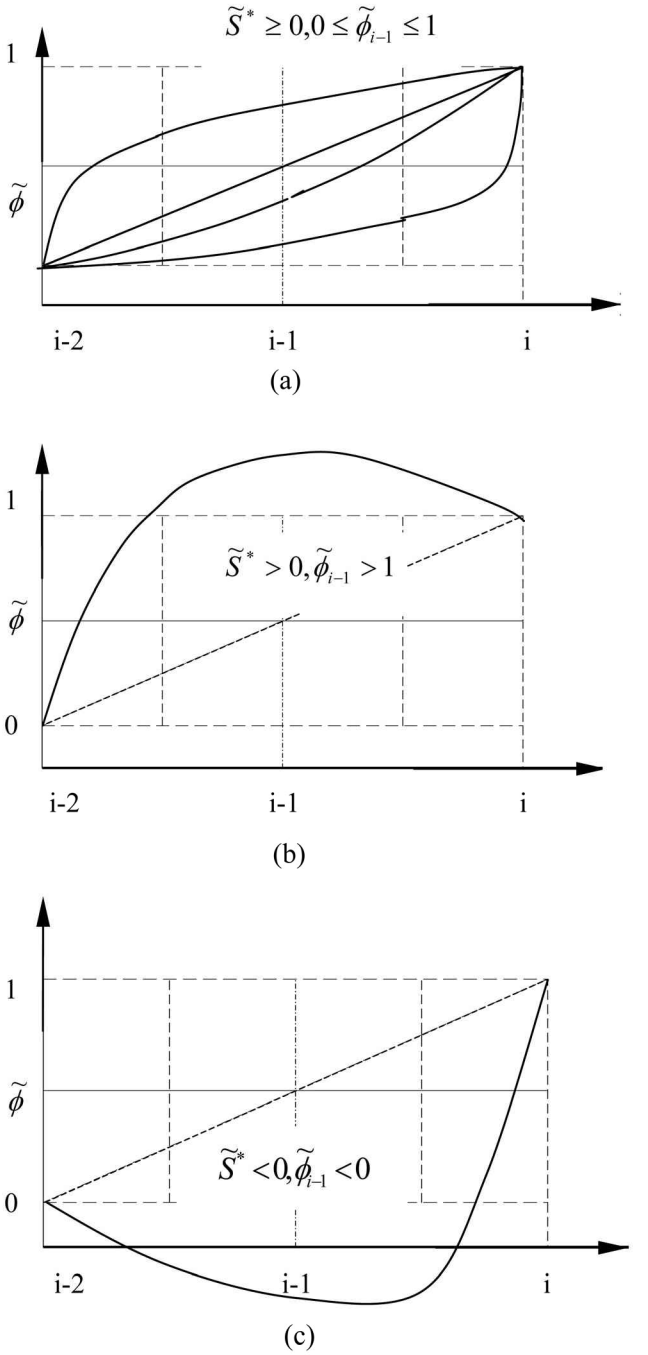


Figure 4.
Realistic profiles of $\tilde{\phi}$ across three successive grid points

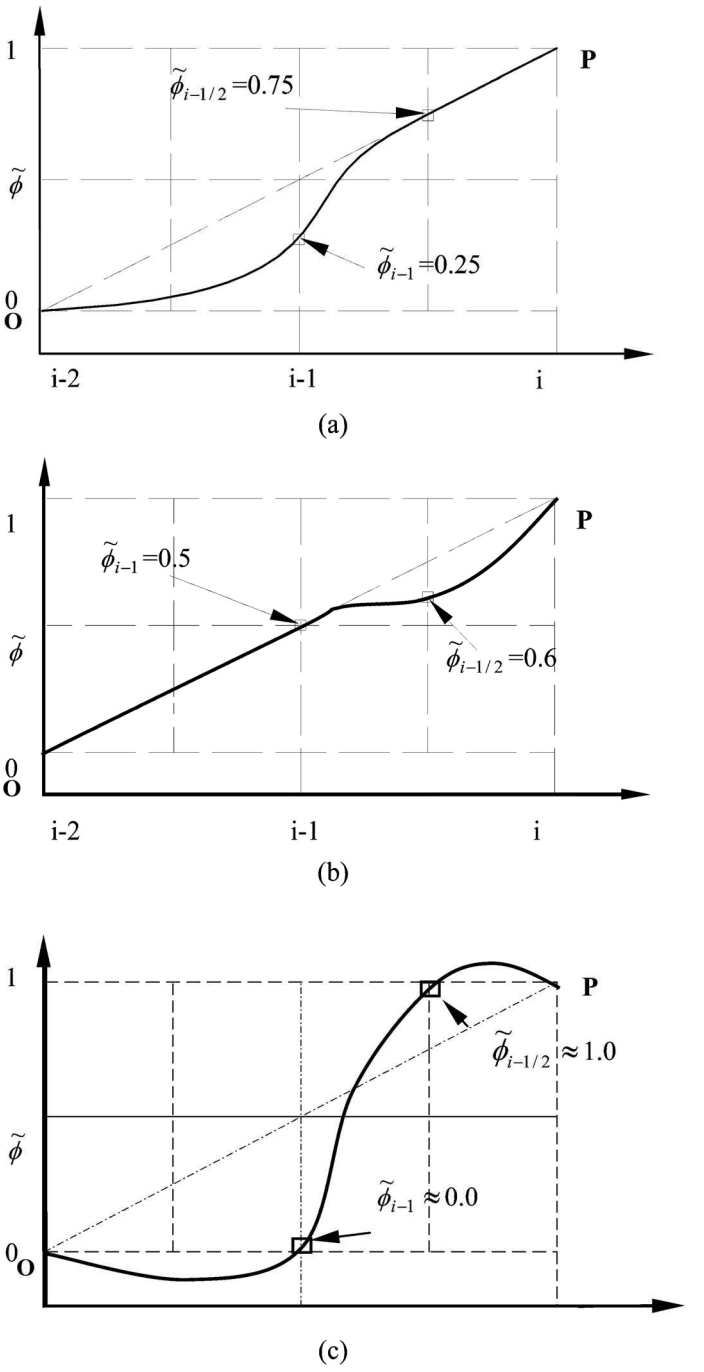


Figure 5.
Unrealistic curves of $\tilde{\phi}$ variations for points A and B

Thus, it become clear that in order to get reasonable variation pattern of the normalized variable, it is necessary to have a more rigorous restrictions on the interface interpolation rules.

Before going into detail discussion on the refinement of CBC, it is worth mentioning the necessity and sufficiency of the GL-CBC. As indicated earlier, there are different point of views about whether GL-CBC is a sufficient and necessary condition for boundedness or not. Actually, GL-CBC is a criterion composed of a series of conditions in different range of $\tilde{\phi}_{i-1}$. Thus, it is reasonable to discuss whether each condition is a sufficient and necessary one for boundedness or not. It will be shown later that the first and second conditions of equation (8) are only sufficient for boundedness, while the third condition is both necessary and sufficient for a scheme to possess boundedness. The necessity can be found easily from NVD: if in the region of $\tilde{\phi}_{i-1} \in [0, 1.0]$, the value of $\tilde{\phi}_{i-1/2}$ is greater than 1.0 or less than 0, the scheme will not possess the boundedness. In this region, the sufficiency is obvious if the interfacial value is located within the shaded area of Figure 1.

3. More rigorous restrictions on the interface interpolation rules

Let us analyze the restrictions on the interface value interpolation from equation (7) and the smoothness requirement of the variable variation pattern. It is important to bear in mind that among the three points of $i-2$, $i-1$ and i, the values of $\tilde{\phi}$ at $i-2$ and i are always fixed (i.e. 0 and 1, respectively), and what we are searching for is the reasonable variation pattern of $\tilde{\phi}$ between the point $i-2$ and i for different values of $\tilde{\phi}_{i-1}$. No matter how large the effective source term $\tilde{S}^*$ is, the resulting final variation pattern of $\tilde{\phi}$ should obey the same rule. Therefore in the following, discussion will be conducted for different values of $\tilde{\phi}_{i-1}$.

3.1 $\tilde{\phi}_{i-1} > 1$

Taking any point, say K, at the vertical line going through $i-1$ and positioned beyond $\tilde{\phi}_{i-1} = 1$ (Figure 6(a)), and making a horizon through K and a straight line going through K and P, we then obtain the suitable region where the variable profile going through the three points O, K and P should be located. This is presented by the thick line shown in Figure 6(a).

The major characteristics of this variation pattern are: from position $i-2$ to $i-1$, the maximum of the curve should be less than $\tilde{\phi}_{i-1}$, and in the region from $i-1$ to i, the curve is located within the triangle region surrounded by the horizon and line PK.

Thus, we obtain the following rule for the interpolation of the interface value:

$$\tilde{\phi}_{i-1/2} \in (0.5(\tilde{\phi}_{i-1} + 1), \tilde{\phi}_{i-1}) \quad \text{for} \quad \tilde{\phi}_{i-1} > 1 \tag{9}$$

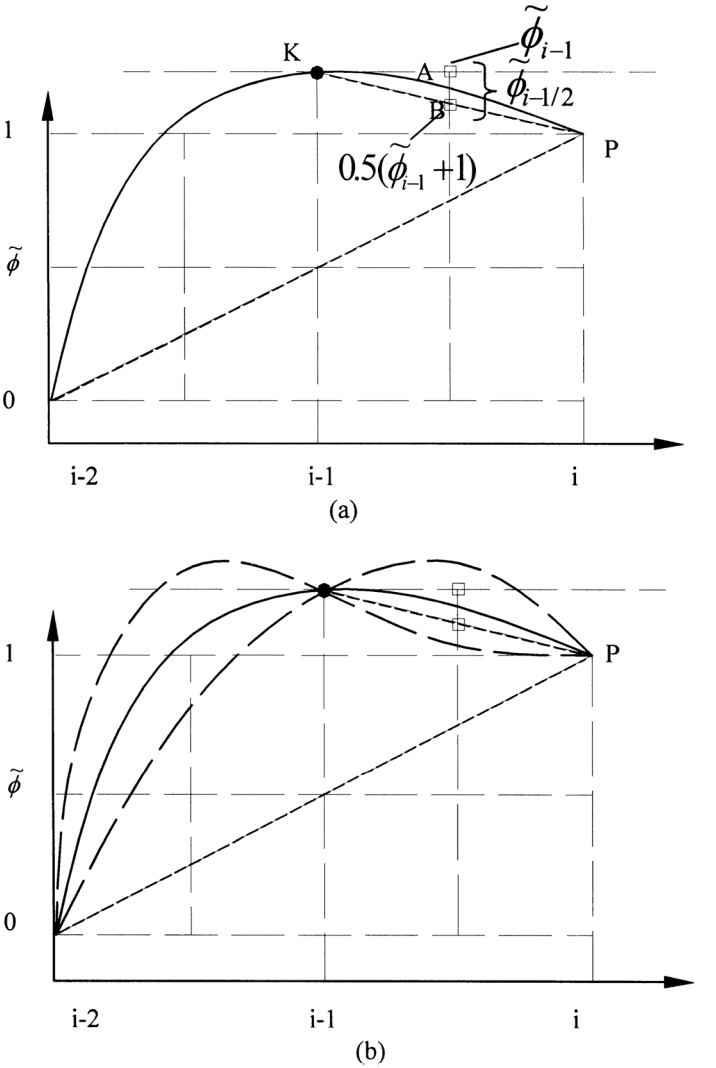


Figure 6.
Diagrammatic analysis of the profiles of $\tilde{\phi}$ for $\tilde{\phi}_{i-1} > 1$

Profiles which violate the above rule are shown by the dashed lines in Figure 6(b). Clearly, neither of them possesses the boundedness character.

3.2 $\tilde{\phi}_{i-1} \in (0.5, 1.0]$

Let us consider any point, say K, within the region of (0.5, 1.0) at the vertical line going through $(i-1)$, and connect points O and K by a straight line OL (Figure 7(a)), and connect the point K and point P to form another straight line KP. A reasonable variation profile of $\tilde{\phi}$ which goes through three points P, K and O should be as follows: from $(i-2)$ to $(i-1)$ its value should not be higher

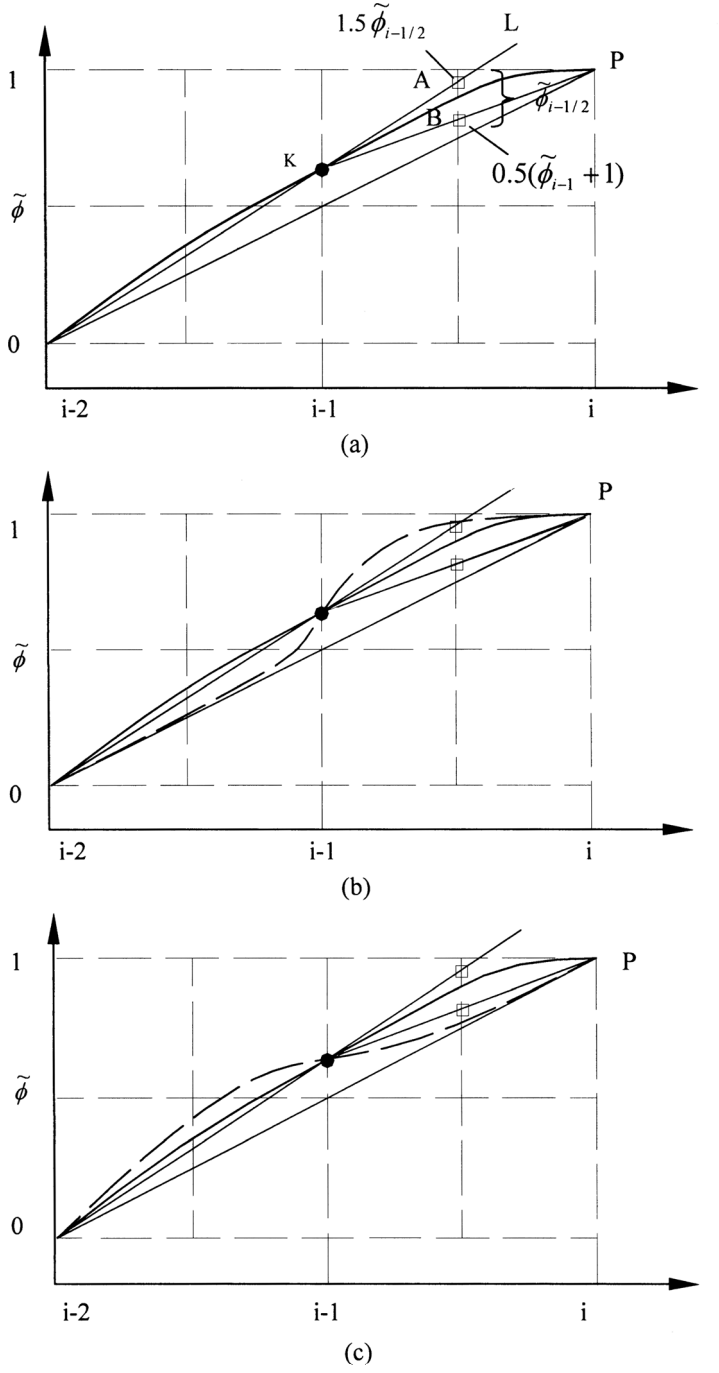


Figure 7. Diagrammatic analysis of the profiles of $\tilde{\phi}$ for $0.5 < \tilde{\phi}_{i-1} \leq 1$

than $\tilde{\phi}_{i-1}$, and from $(i-1)$ to i, the curve should be located between OL and PK. Such a profile is shown in Figure 7(a) by the thick line. Curves which do not abide by the above rules are presented in Figure 7(b) and (c) by the dashed lines. Obviously, curves shown in Figure 7(b) and (c) are not acceptable. From Figure 7(a), we obtain the following interface interpolation rule:

$$\tilde{\phi}_{i-1/2} \in (0.5(\tilde{\phi}_{i-1} + 1), 1.5\tilde{\phi}_{i-1}) \quad \text{for} \quad \tilde{\phi}_{i-1} \in (0.5, 2/3) \tag{10a}$$

In the region of $\tilde{\phi}_{i-1} \in [2/3, 1]$, $1.5\,\tilde{\phi}_{i-1}$ will be larger than 1. To make the interpolation bounded, the following part should be added:

$$\tilde{\phi}_{i-1/2} \in (0.5(\tilde{\phi}_{i-1} + 1), 1) \quad \text{for} \quad \tilde{\phi}_{i-1} \in [2/3, 1.0] \tag{10b}$$

Similar discussion can be made for the other region of $\tilde{\phi}_{i-1}$. In the following, only the figures are presented and the related description is omitted for simplicity.

3.3 $\tilde{\phi}_{i-1} \in [0,0.5]$(Figure 8(a))

$$\tilde{\phi}_{i-1/2} \in (1.5\tilde{\phi}_{i-1},\ 0.5(\tilde{\phi}_{i-1} + 1)), \quad \text{for} \quad \tilde{\phi}_{i-1} \in [0, 0.5] \tag{11}$$

In Figure 8(b) and (c), the curves (dashed lines), which are positioned outside the above region, show unreasonable variations.

3.4 $\tilde{\phi}_{i-1} < 0$ (Figure 9)

It can be seen that a reasonable variation should satisfy the following condition (see the thick line in Figure 9): $\tilde{\phi}_{i-1} < \tilde{\phi}_{i-3/2} < 0.5(\tilde{\phi}_{i-1} + 0)$. Thus, we have:

$$\tilde{\phi}_{i-1} < \tilde{\phi}_{i-3/2} < 0.5\tilde{\phi}_{i-1}, \quad \text{for} \quad \tilde{\phi}_{i-1} < 0 \tag{12}$$

4. New CBC region based on the above discussion

A new CBC criterion based on the above discussion may be constructed as follows: for a continuous or piecewise continuous function $\tilde{\phi}_{i-1/2} = f(\tilde{\phi}_{i-1})$, if the following conditions are satisfied, the scheme represented by $f(\tilde{\phi}_{i-1})$ possesses boundedness with high accuracy:

$$\begin{aligned}
&\text{for } \tilde{\phi}_{i-1} \in (1, +\infty), f(\tilde{\phi}_{i-1}) \in (0.5(1 + \tilde{\phi}_{i-1}), \tilde{\phi}_{i-1}];\\
&\text{for } \tilde{\phi}_{i-1} \in (-\infty, 0), f(\tilde{\phi}_{i-1}) \in [\tilde{\phi}_{i-1}, 0.5\tilde{\phi}_{i-1});\\
&\text{for } \tilde{\phi}_{i-1} \in [0, 0.5), f(\tilde{\phi}_{i-1}) \in (1.5\tilde{\phi}_{i-1}, 0.5(1 + \tilde{\phi}_{i-1})];\\
&\text{for } \tilde{\phi}_{i-1} \in (1/2, 2/3), f(\tilde{\phi}_{i-1}) \in [0.5(1 + \tilde{\phi}_{i-1}), 1.5\tilde{\phi}_{i-1});\\
&\text{for } \tilde{\phi}_{i-1} \in [2/3, 1], f(\tilde{\phi}_{i-1}) \in (0.5(1 + \tilde{\phi}_{i-1}), 1]
\end{aligned} \tag{13}$$

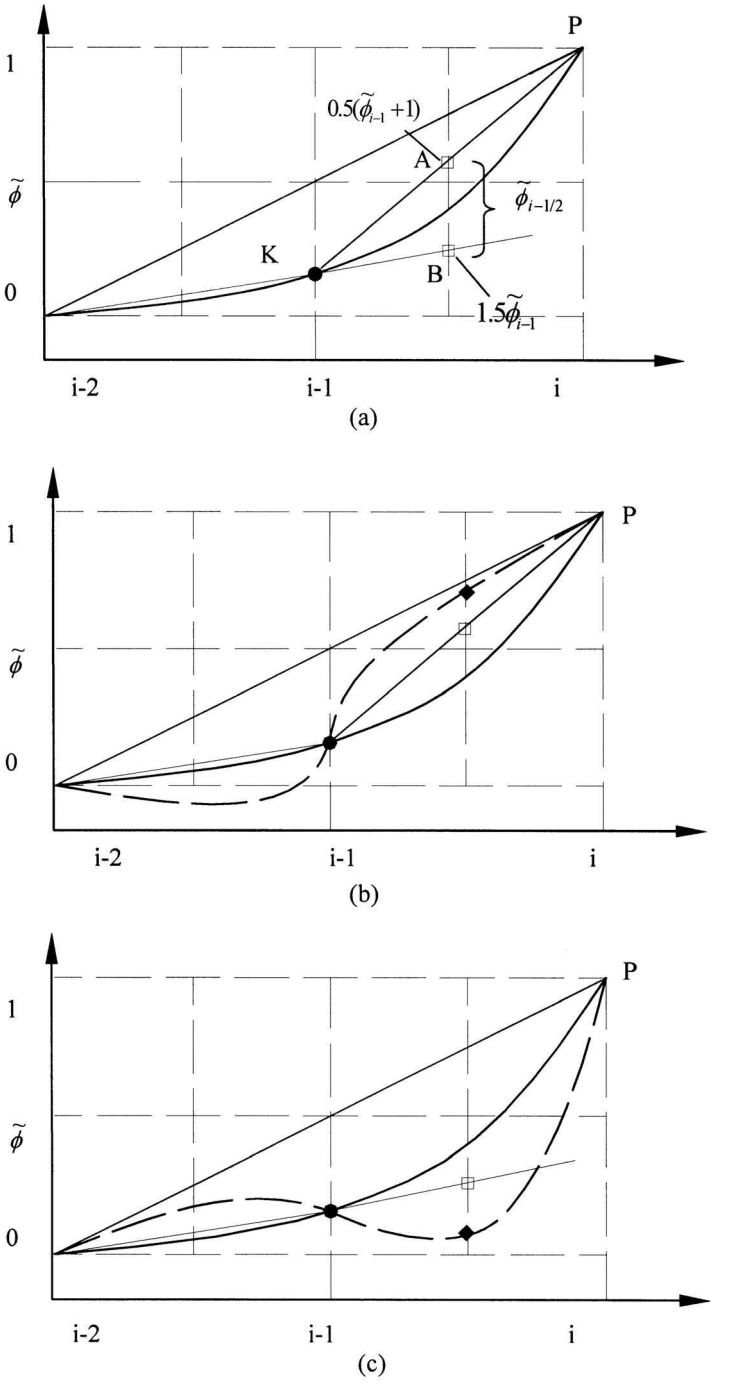


Figure 8. Diagrammatic analysis of the profiles of $\tilde{\phi}$ for $0 \leq \tilde{\phi}_{i-1} \leq 0.5$

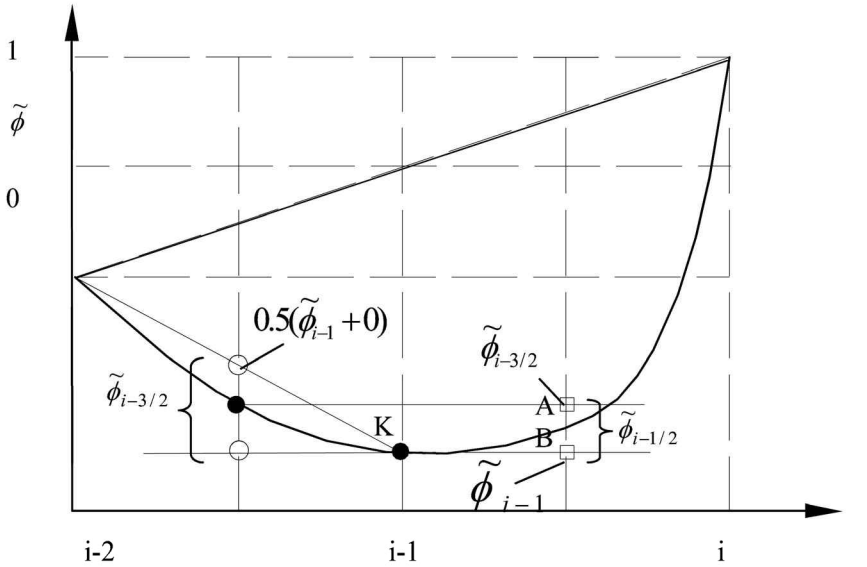


Figure 9.
Diagrammatic analysis of the profiles of $\tilde{\phi}$ for $\tilde{\phi}_{i-1} < 0$

This criterion is shown in Figure 10 by the shaded area. As indicated earlier, the shaded area outside the region of $\tilde{\phi}_{i-1} \in [0, 1]$ coincide with the corresponding area of ECBC proposed by Tao (2000) and Yu *et al.* (2001). The first and second conditions of equation (13) show that the first and second conditions of GL-CBC are only sufficient condition for boundedness.

4.1 Comparative discussion of existing bounded composite schemes

It is interesting to note that in the above analysis, the major requirement posed to the interface interpolation is the profile smoothness of the dependent variable, nothing has been proposed from the point view of truncation error of the interface interpolation. However, the resulting CBC in the NVD has a very unique feature: it goes through point Q (0.5, 0.75). As proved by Leonard (1991), any scheme whose characteristic line goes through point Q (0.5, 0.75) (Figure 10) possesses at least second-order accuracy. Therefore, we conclude that the newly-proposed CBC area is the collection of all possible composite schemes whose accuracy is atleast of second-order.

The examination of the new CBC for the existing ten bounded convective schemes are conducted, including the most-recently proposed one (WACEB). For the compactness of presentation, the definitions of these schemes are shown in Figure 11, where the corresponding characteristic lines are also drawn. All the ten schemes are claimed to have atleast second-order of accuracy, and their characteristic line all go through point Q, showing the

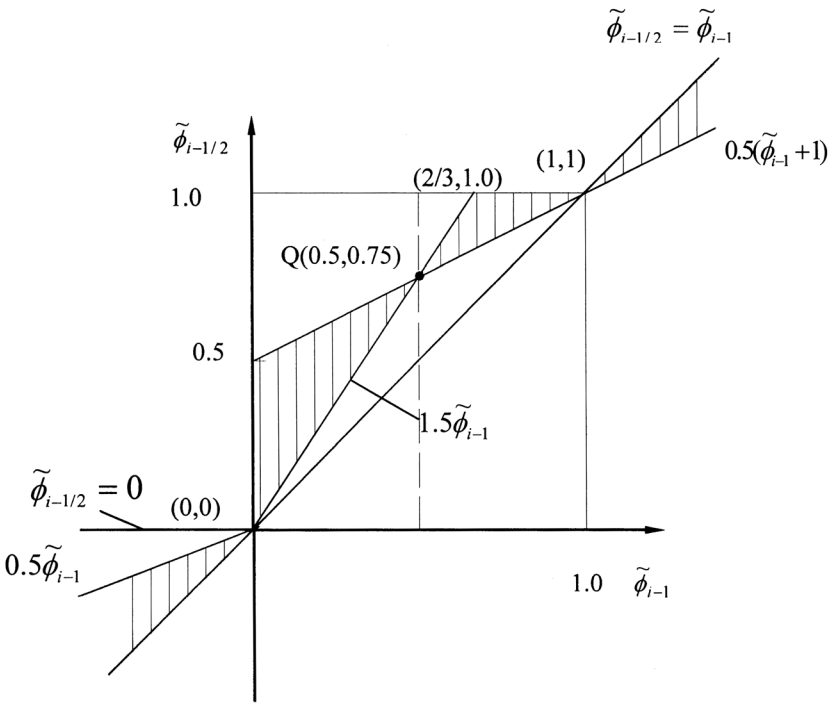


Figure 10.
Representation of refined CBC

correctness of the analysis presented by Leonard (1991) and Tao (2000). The most surprising finding is that the characteristic lines of the ten schemes are all located within this new CBC region, giving a strong support of the above analysis. It is worth noting that when the first version of the manuscript was prepared, the present authors were not aware of WACEB (Song *et al.*, 2000). We found it during the revision of our paper. This scheme was constructed from very different point of view. Based on several existing high-order schemes, Song *et al.* (2000) proposed the following general normalized form of the interfacial variable:

$$\tilde{\phi}_f = \tilde{\phi}_C + 1/4[(1+\kappa)(1-\tilde{\phi}_C) + (1-\kappa)\tilde{\phi}_C] \tag{14}$$

where κ is called the weighted average coefficient. They obtained κ from the requirement of boundedness and TVD, and derived a complicated dependency of κ with $\tilde{\phi}_C$. The resulting definition of the scheme is cited in Figure 11 of the present paper. The characteristic line of WACEB also fall in the region of our new CBC, further demonstrating the feasibility of the present new CBC.

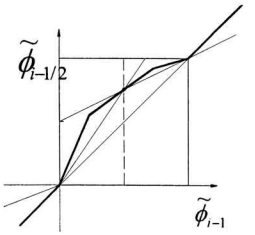
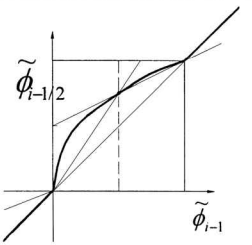
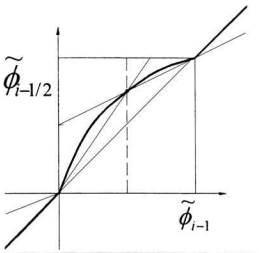
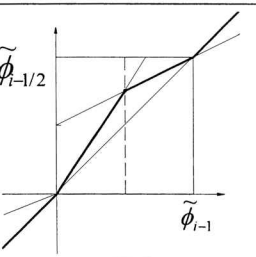
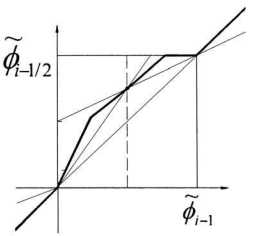
No	Scheme	Definition with Normalized Variable	Normalized Variable Diagram
1 [10]	COPLA (combination of piecewise linear approximation)	$\tilde{\phi}_{i-1/2} = 2.25\tilde{\phi}_{i-1} \quad 0 \le \tilde{\phi}_{i-1} \le 1/4$ $= \frac{3}{8} + \frac{3}{4}\tilde{\phi}_{i-1} \quad \frac{1}{4} \le \tilde{\phi}_{i-1} \le \frac{3}{4}$ $= \frac{3}{4} + \frac{1}{4}\tilde{\phi}_{i-1} \quad \frac{3}{4} \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	
2 [11]	EULER	$\tilde{\phi}_{i-1/2} = \frac{\sqrt{\tilde{\phi}_{i-1}(1-\tilde{\phi}_{i-1})^3} - \tilde{\phi}_{i-1}^2}{1-2\tilde{\phi}_{i-1}}, 0 \le \tilde{\phi}_{i-1} \le 1$ $= 3/4 \quad \tilde{\phi}_{i-1} = 0.5$ $= \tilde{\phi}_{i-1} \quad$ *else*	
3 [6]	CLAM (hybrid linear/parabolic approximation)	$\tilde{\phi}_{i-1/2} = \tilde{\phi}_{i-1}(2-\tilde{\phi}_{i-1}) \quad 0 \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	
4 [8]	MINMOD (minimum modulus)	$\tilde{\phi}_{i-1/2} = \frac{3}{2}\tilde{\phi}_{i-1} \quad 0 \le \tilde{\phi}_{i-1} \le \frac{1}{2}$ $= \frac{1}{2}(1+\tilde{\phi}_{i-1}) \quad 0.5 \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	
5 [5]	MUSCL (monotonic upwind scheme for conservation law)	$\tilde{\phi}_{i-1/2} = 2\tilde{\phi}_{i-1} \quad 0 \le \tilde{\phi}_{i-1} \le 1/4$ $= 1/4 + \tilde{\phi}_{i-1} \quad \frac{1}{4} \le \tilde{\phi}_{i-1} \le \frac{3}{4}$ $= 1 \quad \frac{3}{4} \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	

Figure 11.
Existing bounded composite schemes

(*continued*)

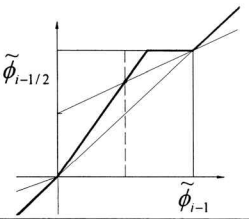
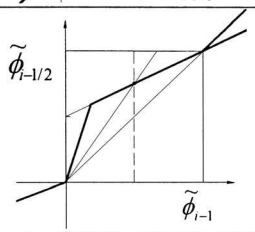
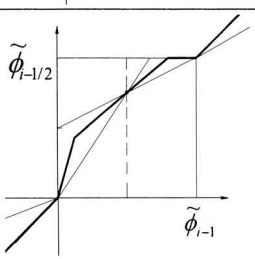
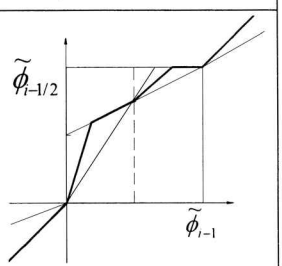
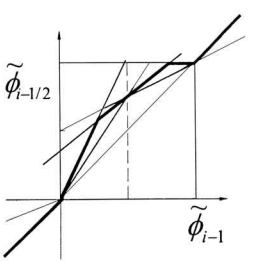
6 [7]	OSHER	$\tilde{\phi}_{i-1/2} = \frac{3}{2}\tilde{\phi}_{i-1}$ $\quad 0 \le \tilde{\phi}_{i-1} \le 2/3$ $= 1 \quad 2/3 \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	
7 [12]	SECBC (scheme based on extended CBC)	$\tilde{\phi}_{i-1/2} = \frac{1}{2}\tilde{\phi}_{i-1}$ $\quad \tilde{\phi}_{i-1} \le 0$ $= 3\tilde{\phi}_{i-1} \quad 0 < \tilde{\phi}_{i-1} < 0.2$ $= \frac{\tilde{\phi}_{i-1}+1}{2} \quad \tilde{\phi}_{i-1} \ge 0.2$	
8 [2]	SMART (sharp and monotonic algorithm for realistic transport)	$\tilde{\phi}_{i-1/2} = 3\tilde{\phi}_{i-1}$ $\quad 0 \le \tilde{\phi}_{i-1} \le 1/6$ $= 3/8 + 3/4\tilde{\phi}_{i-1} \quad \frac{1}{6} \le \tilde{\phi}_{i-1} \le \frac{5}{6}$ $= 1 \quad \frac{5}{6} \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	
9 [9]	STOIC (second and third order interpolation for convection)	$\tilde{\phi}_{i-1/2} = 3\tilde{\phi}_{i-1}$ $\quad 0 \le \tilde{\phi}_{i-1} \le 1/5$ $= 1/2(1+\tilde{\phi}_{i-1}) \quad \frac{1}{5} \le \tilde{\phi}_{i-1} \le \frac{1}{2}$ $= \frac{3}{8} + \frac{3}{4}\tilde{\phi}_{i-1} \quad \frac{1}{2} \le \tilde{\phi}_{i-1} \le \frac{5}{6}$ $= 1 \quad \frac{5}{6} \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	
10 [1]	WACEB (weighted-average coefficient ensuring boundedness)	$\tilde{\phi}_{i-1/2} = 2\tilde{\phi}_{i-1}$ $\quad 0 \le \tilde{\phi}_{i-1} \le 0.3$ $= 3/8 + 3/4\tilde{\phi}_{i-1} \quad 0.3 \le \tilde{\phi}_{i-1} \le \frac{5}{6}$ $= 1 \quad \frac{5}{6} \le \tilde{\phi}_{i-1} \le 1$ $= \tilde{\phi}_{i-1} \quad$ *else*	

Figure 11.

4.2 Numerical comparison between GL-CBC and the new CBC

To further demonstrate the correctness of the proposed new-CBC, two schemes, called scheme 1 and 2, are deliberately designed, which although abide by the GL-CBC rule, do not satisfy the condition represented by equation (13). The definition of scheme 1 is represented by:

$$\begin{aligned}\tilde{\phi}_{i-1/2} &= 9\tilde{\phi}_{i-1} - 8 \quad 0 \le \tilde{\phi}_{i-1} \le 1 \\ &= 1/9\tilde{\phi}_{i-1} - 8/9 \quad 0.1 \le \tilde{\phi}_{i-1} \le 1 \\ &= \tilde{\phi}_{i-1} \quad \text{else}\end{aligned} \tag{15}$$

The second scheme is represented by:

$$\tilde{\phi}_{i-1/2} = \tilde{\phi}_{i-1} \tag{16}$$

The characteristic lines of the two schemes are shown in Figure 12.

The one-dimensional diffusion-convection problem represented by equation (4) is solved by the numerical method with the diffusion term discretized by central difference and the convective term discretized by the two scheme and SMART. The numerical results for grid Peclet number equals 1 and 5 are shown in Figure 13, where the exact solution is also provided for comparison purpose. It can be seen that although the two deliberately proposed schemes get physically plausible solutions, their accuracy is not so good as SMART, indicating that the smoothness of the variation pattern of the dependent variable is of great importance for scheme accuracy.

5. Conclusion

In this paper, refinements to the GL-CBC are made based on a careful consideration of the smoothness of the profile variation pattern of the normalized variable. The new CBC proposed guarantees not only the boundedness, but also high-order of accuracy. Analysis of the requirement of profile smoothness shows that the first and second constraints of GL-CBC are sufficient ones, and the third condition is a necessary and sufficient one for boundedness. The GL-CBC can only guarantee the boundedness, without any accuracy consideration. The new CBC is a sufficient and necessary condition for a bounded scheme to possess at least second-order accuracy. Inspection of the ten existing bounded schemes has shown that all the ten schemes meet the requirement of the new CBC, giving a strong support to the present analysis. Two schemes are deliberately designed which meet the GL-CBC, but not satisfy the newly-proposed CBC. Numerical experiments show that the accuracy of the numerical solutions resulted from the two schemes are inferior to that of SMART, illustrating the importance of the smoothness of the variable profile for scheme accuracy.

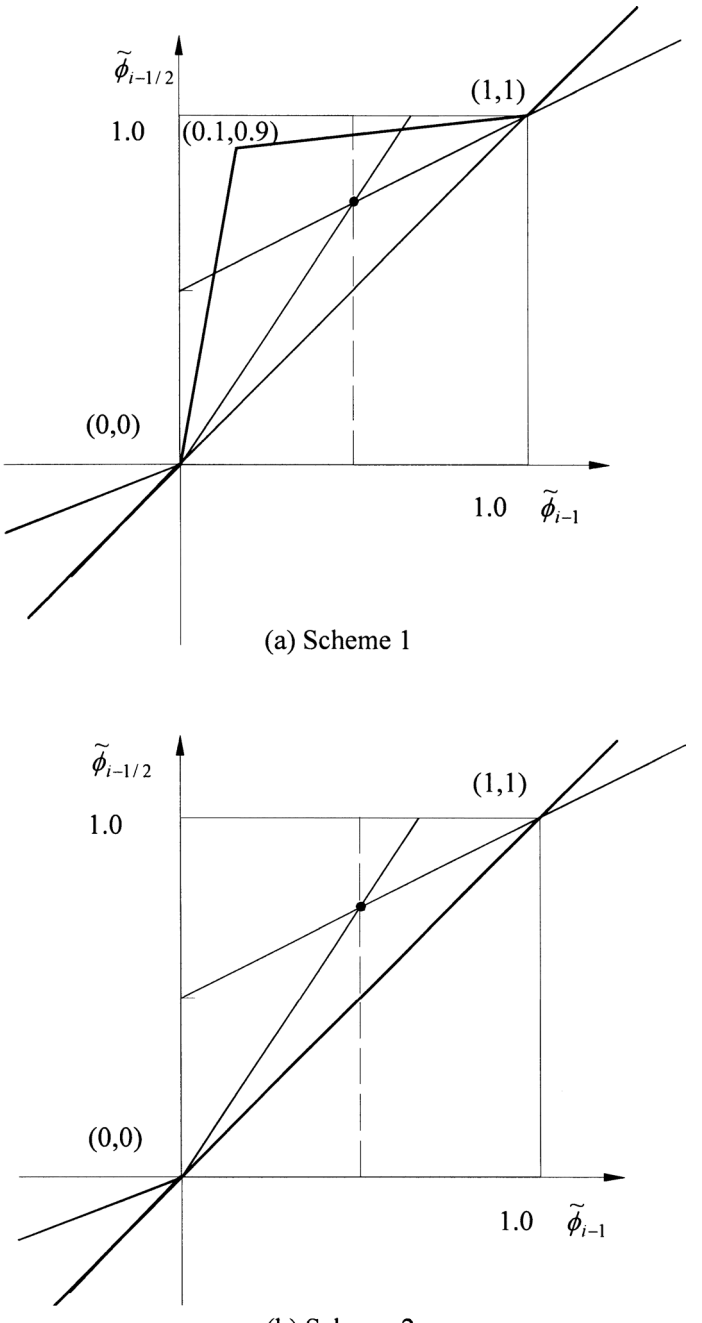
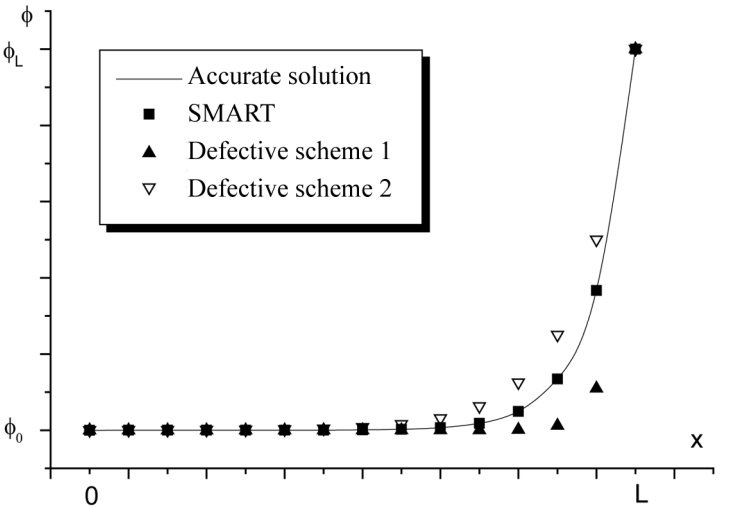
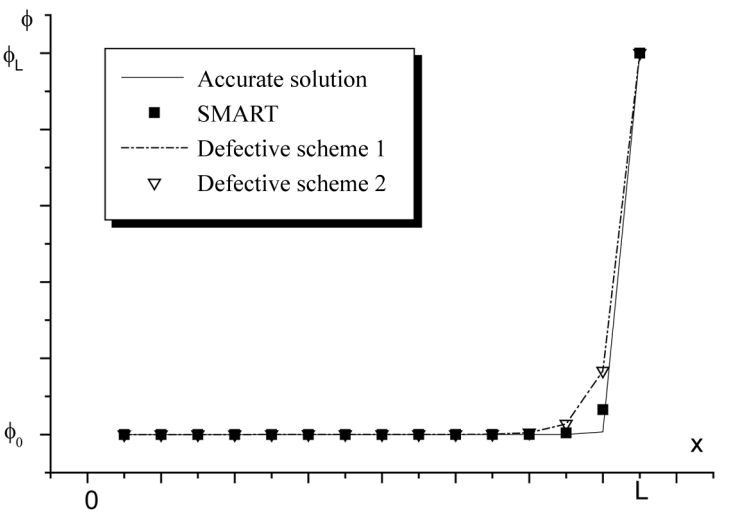


Figure 12. Representation of two deliberately designed schemes



(a) Cell Peclect Number is 1



(b) Cell Peclect Number is 5

Figure 13.
Comparison of the numerical solutions for different cell Peclect numbers

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