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A LOCALLY MODIFIED SECOND ORDER UPWIND SCHEME FOR CONVECTION TERMS DISCRETIZATION

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ABSTRACT

A finite difference scheme for convection term discretization, called *BSOU* (stands for Bounded Second Order Upwind), is developed and its performance is assessed against exact or benchmark solutions in linear and non-linear cases. It employs a flux blending technique between first order upwind and second order upwind schemes only in those regions of the flow field where spurious oscillations are likely to occur. The blending factors are calculated with the aid of the convection boundedness criterion. In all cases the scheme performed very well, minimizing the numerical diffusion errors. The scheme is transportive, conservative, bounded, stable and accurate enough so as to be suitable for inclusion into a general purpose solution algorithm.

KEY WORDS Finite differencing schemes Boundedness property Convection-diffusion problems

NOMENCLATURE

A_E, A_W etc.	Coefficients of finite difference equations
BSOU	Bounded Second Order Upwind
FOU	First Order Upwind
Re	Reynolds number
SOU	Second Order Upwind
TVD	Total Variation Diminishing
u_i	U velocity at cell face i
U, V	Transport velocities in x, y directions respectively.

Greek symbols

γ	Blending factor
Γ_ϕ	Diffusivity
ΔX_{ij}	Distance between i, j in direction x
ΔY_{ij}	Distance between i, j in direction y
ρ	Density
ϕ	General transported variable
$\tilde{\phi}$	Normalized variable
ϕ_i	Value of ϕ at cell face i

INTRODUCTION

It is well known that numerical diffusion errors, caused by the use of first order upwind scheme (referred to as *FOU* below) for the discretization of the convection terms of transport equations, can impart significant errors to fluid flow predictions, especially when associated with significant skewness between velocity and grid lines, see for example Huang *et al.*[1]. The approaches used to remedy the problem are mesh refinement and adoption of finite difference schemes with a higher formal order of accuracy than *FOU*.

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Mesh refinement is feasible to apply in two dimensional plane or axisymmetric problems, but is difficult to employ in three dimensional problems; especially when, beside the equations which describe turbulent flow fields, additional equations modelling complex physical phenomena (combustion, heat transfer, radiation etc.) are to be solved.

Schemes with higher order truncation errors than *FOU* have been proposed and employed as an alternative in an attempt to remedy the numerical diffusion problem. The desired properties such schemes must have are: transportiveness (when convection becomes more dominant than diffusion, upstream nodes have more influence than downstream ones); conservativeness (when the flux across any cell face is uniquely determined for the two adjacent control volumes), boundedness (when in the absence of any source term, the grid node values remain between the minimum and maximum boundary values) and accuracy. The combination of these properties is not an easy task, since they are contradictory to each other. For example, higher order schemes are capable of reducing numerical diffusion errors (high accuracy), but they are susceptible to numerical instabilities (violation of boundedness property), making the convergence of the whole iteration procedure for Navier–Stokes solution, very difficult or even, sometimes, impossible.

Two of the higher order schemes, that have been used the most in the literature, are the *QUICK* scheme of Leonard[2] and the second order upwind scheme (referred to as *SOU* below). Curve fitting methods are used to approximate the cell face values: linear polynomial for *SOU* and quadratic for *QUICK*. Both schemes have higher formal order of accuracy than *FOU*; 3rd order for *QUICK* and 2nd order for *SOU*. Both violate the boundedness property. In a comparative study between the two schemes, several investigators (Shyy[3], Castro and Jones[4]) have found that *SOU* is considered better when judged with respect to accuracy and computational stability.

Accuracy is greatly affected by the way the scheme is implemented in a computational code. Shy *et al.*[5] have compared three versions of the *SOU* scheme (all having the same formal order of accuracy) and found that the best results are obtained when the conservative version of *SOU* is implemented in a way consistent with the control volume formulation. Vanka[6], on the other hand, found that the *SOU* scheme does not yield satisfactory accuracy when solving the two-dimensional cavity flow problem for several Reynolds numbers and finite difference grids. He, however, employed a non-conservative version of the scheme.

In the flux-spline method of Varejao[7], the distribution of the dependent variable is not determined by curve fitting polynomials. It is obtained by solving a simplified form of the governing equation which is based on the assumption that within a control volume the total convection and diffusion flux varies in a piece wise linear manner. The resulting variation of the dependent variable contains an exponential term and a linear term. The scheme has been tested in a number of test cases (Varejao[7]) and found to give accurate results. It, however, violates the boundedness property.

The presence of wiggles (overshoots and undershoots), indicate that the employed numerical grid is not fine enough to properly resolve local steep gradients of the transported variable. Gresho *et al.*[8] point out that wiggles may even be looked upon as an advantage since at least they give an indication on the location of the flow field where the mesh cannot resolve the steep gradients and subsequently suggest the regions where local refinement is necessary in order to eliminate wiggles. On the other hand, a diffusive solution does not give a clear indication of the critical regions of the flow, unless a method is employed to access the local numerical diffusion error a posteriori, as is done by McGuirk *et al.*[9]. However, the boundedness of the solution is a very important characteristic since it enhances convergence and it enables the scheme to be used to all transport equations including turbulence kinetic energy, its dissipation rate, species concentrations, enthalpy etc. whose values must always be positive. Use of unbounded schemes cause unrealistic negative values for these quantities.

Several methods exist which remove spurious oscillations from the solutions of higher order schemes and thus account for the boundedness property. For steady state calculations of incompressible flows, the flux blending technique (documented in Benodekar *et al.*[10]) and the satisfaction of the convection boundedness criterion (Gaskell and Lau[11], Leonard and Niknafs[12]) are the two most widely used methods. For example, in the *LODA* scheme of Zhu and Leschziner[13], a flux blending technique is employed between *QUICK* and *FOU* in order to obtain a bounded version of *QUICK*. Similarly, Peric[14] has developed a flux blending technique, which he employed to *QUICK* and *SOU*. On the other hand Gaskell and Lau[11] used the convection boundedness criterion in order to construct the *SMART* scheme, which effectively removes over- and undershoots from *QUICK*. Zhu and Rodi[15] developed the *SOUCUP* scheme, which is essentially a combination of *FOU*, central difference and *SOU*, with the switch from one scheme to the other being controlled by the convection boundedness criterion.

For explicit time marching algorithms (used especially for compressible flows), the *F.C.T.* (Flux Corrected Transport) method of Boris and Book[16] and Zalesak[17] or the *F.R.A.M.* (Filtering Remedy and Methodology) algorithm of Chapman[18] have been used. Sharif and Busnaina[19] have used both the *F.C.T.* and *F.R.A.M.* methods to eliminate oscillations from the skew upwind scheme of Raithby[20] and from the *SOU* scheme. The *F.C.T.* algorithm effectively treats the dispersion problem for both schemes but the *F.R.A.M.* method fails when employed to the *SOU* scheme.

Finally, schemes that have *T.V.D.* (Total Variation Diminishing) properties are also monotonicity preserving schemes (Harten[21]). Sweby[22] introduced sufficient conditions for schemes to have such properties and portrayed these conditions on the Sweby diagram. The close relationship between the Sweby *T.VD.* diagram and the convection boundedness criterion are presented by Leonard[23]. Based on this similarity, the *SOUCUP* scheme of Zhu and Rodi[15] is identical to the Roe's *T.V.D.* minmod scheme in the steady state case.

The scope of the present paper is to propose a method which combines the flux blending technique (between *SOU* and *FOU*) and the convection boundedness criterion for the production of a wiggle free scheme, which is called *BSOU*. The scheme is formulated so that it can be directly applicable to algorithms for incompressible flows.

In what follows, a description of the mathematical formulation of the *BSOU* scheme is given, its relation to existing *T.V.D.* schemes is discussed and results are presented, from 3 test cases, which illustrate the scheme's performance in simple and complex flows.

MATHEMATICAL FORMULATION. DIFFERENTIAL EQUATIONS AND DISCRETIZATION

The general form of transport equation of variable ϕ in two-dimensional Cartesian system is:

$$\frac{\partial}{\partial x}(\rho U\phi) + \frac{\partial}{\partial y}(\rho V\phi) - \frac{\partial}{\partial x}\left(\Gamma_\phi \frac{\partial \phi}{\partial x}\right) - \frac{\partial}{\partial y}\left(\Gamma_\phi \frac{\partial \phi}{\partial y}\right) = S_\phi \tag{1}$$

where U, V are the transport velocities in the x, y direction respectively, Γ_ϕ is the diffusivity and S_ϕ denotes the source term.

The discretized form of equation (1) is deduced by integration over the control volume shown in *Figure 1*, and assumes the form:

$$\left[\rho U\phi - \Gamma_\phi \frac{\partial \phi}{\partial x}\right]_e \Delta Y_{sn} - \left[\rho U\phi - \Gamma_\phi \frac{\partial \phi}{\partial x}\right]_w \Delta Y_{sn} + \left[\rho V\phi - \Gamma_\phi \frac{\partial \phi}{\partial y}\right]_n \Delta X_{we} - \left[\rho V\phi - \Gamma_\phi \frac{\partial \phi}{\partial y}\right]_s \Delta X_{we} = S_\phi * Vol \tag{2}$$

where each quantity inside the brackets is calculated on the corresponding face of the control volume.

The calculation of the derivative $\partial\phi/\partial x$, $\partial\phi/\partial y$ etc. is made using central differences, i.e.:

$$\left.\frac{\partial\phi}{\partial x}\right|_e = \frac{\phi_E - \phi_P}{\Delta X_{PE}} \tag{3}$$

As far as approximation of the cell face values of variable ϕ is concerned, several alternatives exist. For example for the FOU scheme:

$$\phi_e^{FOU} = \begin{cases} \phi_P & \text{if} \quad u_e > 0 \\ \phi_E & \text{if} \quad u_e < 0 \end{cases} \tag{4}$$

i.e. the cell face value is equal to the upstream value, while for the SOU scheme:

$$\phi_e^{SOU} = \begin{cases} \phi_P + (\phi_P - \phi_W)\Delta X_{Pe}/\Delta X_{WP} & \text{if} \quad u_e > 0 \\ \phi_E + (\phi_E - \phi_{EE})\Delta X_{eE}/\Delta X_{E-EE} & \text{if} \quad u_e < 0 \end{cases} \tag{5}$$

i.e. the cell face value is calculated from linear extrapolation of the two upstream values. Similar approximations hold for the rest of the cell face values.

Substituting (3) and (4) or (5) along with their counterparts for the other cell faces, into (2), the finite difference equations for SOU and FOU are obtained, respectively.

The SOU yields unbounded solutions while FOU is unconditionally bounded. In the next paragraph, a method which combines the two schemes and yields monotone solutions at an insignificant penalty to SOU's non diffusive characteristics, is presented.

DEVELOPMENT OF THE *BSOU* SCHEME

The $BSOU$ scheme relies on the convection boundedness criterion. A brief description will now be given for that criterion.

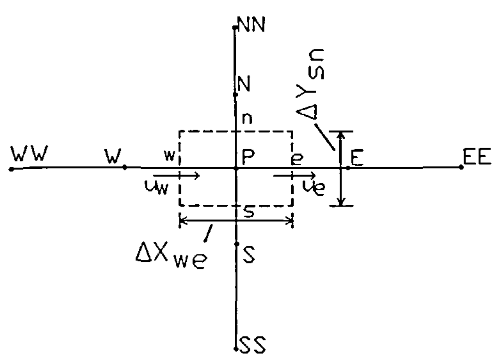


Figure 1 Scheme of the control volume

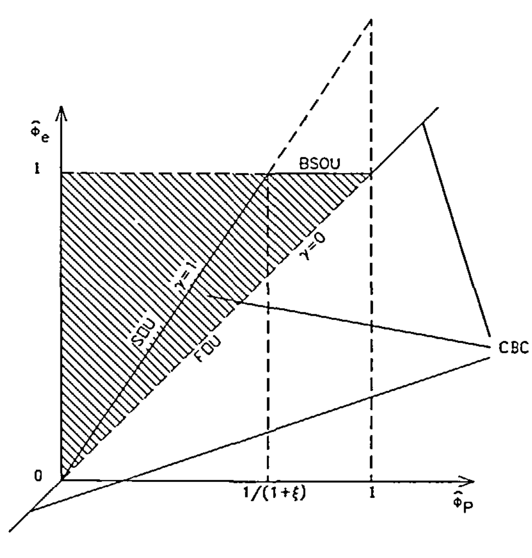


Figure 2 Graphic representation of the convection boundedness criterion (CBC) and the $BSOU$ scheme in the $[\hat{\Phi}_P, \hat{\Phi}_e]$ plane

Consider the control volume surrounding the point P in *Figure 1*. Assuming $u_e > 0$, the normalized variable $\hat{\phi}$ is defined as:

$$\hat{\phi}_k = \frac{\phi_k - \phi_W}{\phi_E - \phi_W}, \qquad k = W, w, P, e, E \tag{7}$$

Each scheme is presented in the plane $[\hat{\phi}_P, \hat{\phi}_e]$ by the function $\hat{\phi}_e = f(\hat{\phi}_P)$. If f is a continuous increasing function, the scheme is bounded if:

(a) for $\hat{\phi}_P \in [0, 1] f(\hat{\phi}_P) \leqslant 1$ and $f(\hat{\phi}_P) \geqslant \hat{\phi}_P$, $f(0) = (0)$, $f(1)1 = 1$.
(b) for $\hat{\phi}_P \notin [0, 1] f(\hat{\phi}_P) = \hat{\phi}_P$.

The scheme is shown diagrammatically in *Figure 2*. The line $\hat{\phi}_e = \hat{\phi}_P$ and the shaded area are the regions where the criterion is valid.

The *SOU* in normalized variables is expressed as:

$$\hat{\phi}_e^{SOU} = (1 + \xi)\hat{\phi}_P \tag{7a}$$

where $\xi = \Delta X_{Pe}/\Delta X_{WP}$, while the *FOU* as:

$$\hat{\phi}_e^{FOU} = \hat{\phi}_P \tag{7b}$$

Simple inspection of *Figure 2* reveals that the *SOU* scheme satisfies the criterion only when $\hat{\phi}_P \in [0, 1/(1 + \xi)]$, while outside this region the criterion is not fulfilled. Thus problems appear in the region $[1/(1 + \xi), 1]$ where $\hat{\phi}_e > 1$. It is in this region, where the blending factors γ, between *SOU* and *FOU* are introduced. The idea behind the blending factors is simple: at each cell face, the resultant flux is obtained by blending the flux obtained from a low order unconditionally bounded scheme (*FOU*) with the flux determined from a higher order, but more accurate scheme (in this case *SOU*). The question to be answered is how the local value of γ is to be determined for each cell face. This is done simply by letting:

$$\begin{aligned}
&\gamma_e \hat{\phi}_e^{SOU} + (1 - \gamma_e)\hat{\phi}_e^{FOU} = 1 \Rightarrow \\
&\gamma_e \hat{\phi}_P(1 + \xi) + (1 - \gamma_e)\hat{\phi}_P = \Rightarrow (1 + \gamma_e \xi)\hat{\phi}_P = 1 \Rightarrow \\
&\gamma_e = \frac{(1/\hat{\phi}_P - 1)}{\xi}
\end{aligned} \tag{8}$$

This is the equation that is used to calculate the blending factor, γ_e for the face e, in such a way that the resulting scheme is always bounded. Graphic representation of the scheme in $[\hat{\phi}_P, \hat{\phi}_e]$ plane is shown in *Figure 2*. This representation reveals that in the steady state case, *BSOU* is identical to the Chakravarthy–Osher[23] scheme and the *ULTIMATE*-Second Order Upwind of Leonard[23]. However, while the two previous schemes are applicable only to time marching procedures (used mainly for compressible flow calculations), the present scheme is directly applicable to *TEACH*-like procedures which are extensively used in the area of incompressible flow calculations.

Concluding, $\hat{\Phi}_e$ is given by the following formula:

$$\hat{\Phi}_e^{BSOU} = \begin{cases} \hat{\Phi}_P & \text{for } \hat{\Phi}_P < 0 \\ (1 + \xi)\hat{\Phi}_P & \text{for } 0 < \hat{\Phi}_P < 1/1 + \xi \\ (1 + \gamma_e \xi)\hat{\Phi}_P & \text{for } 1/1 + \xi < \hat{\Phi}_P < 1 \\ \hat{\Phi}_P & \text{for } \hat{\Phi}_P > 1 \end{cases} \tag{9}$$

For $\gamma_e = 0$ the scheme reduces to *FOU* while for $\gamma_e = 1$ the scheme becomes *SOU*. The blending factors are automatically adjusted during the iteration process and are evaluated only in those regions of the flow field where spurious oscillations are likely to occur.

It is evident from the previous analysis that the resulting scheme is non-linear; for the γ_e calculation one must already know $\hat{\Phi}_P$. It is for this reason that, even for linear problems, it is necessary to perform an iterative process for convergence. The non-linearity may also need the introduction of under-relaxation in order to obtain a converged solution.

The form of the finite difference equations for the *BSOU* scheme is:

$$A_P \Phi_P = A_E \Phi_E + A_W \Phi_W + A_N \Phi_N + A_S \Phi_S + A_{EE} \Phi_{EE} + A_{WW} \Phi_{WW} + A_{NN} \Phi_{NN} + A_{SS} \Phi_{SS} + SU \tag{10}$$

where:

$$A_P = A_E + A_W + A_N + A_S + A_{EE} + A_{WW} + A_{NN} + A_{SS}$$

$$A_{WW} = -\max(0, CW \times \Delta X_{Ww}/\Delta X_{WW-w} \times \gamma_w)$$

$$A_{EE} = -\max(0, -CE \times \Delta X_{eE}/\Delta X_{e-EE} \times \gamma_e)$$

$$A_W = \max(0, CW \times (1 + \Delta X_{Ww}/\Delta X_{WW-w} \times \gamma_w)) + \max(0, CE \times \Delta X_{Pe}/\Delta X_{WP} \times \gamma_e) + DW$$

$$A_E = \max(0, -CE \times (1 + \Delta X_{eE}/\Delta X_{e-EE} \times \gamma_e)) + \max(0, CW \times \Delta X_{wP}/\Delta X_{PE} \times \gamma_w) + DE$$

where:

$$DW = [\Gamma_\Phi]_w \Delta Y_{sn}/\Delta X_{WP}, \qquad DE = [\Gamma_\Phi]_e \Delta Y_{sn}/\Delta X_{PE}$$

$$CW = [\rho u]_w \Delta Y_{sn}, \qquad CE = [\rho u]_e \Delta Y_{sn}$$

Similar equations also hold for the rest of the coefficients. The coefficients of the most distant nodes are always non-positive (zero for downstream nodes and negative for upstream ones), while the 'principal' coefficients are always positive and diagonal dominance exists. The matrix of the finite difference equations can be cast in the well known five diagonal form if the terms involving the remote nodes are incorporated into the source term. In this way, the system can be solved by standard iterative techniques like *ADI*.

Since the scheme involves 5 points in each direction (x, y), special treatment must be given to grid nodes near the boundary planes. In the present study, the *FOU* approximation was applied to all boundaries. This was done because of ease of implementation (simply by setting the blending factor equal to zero) and because boundary conditions of higher order, although having increased accuracy, cause numerical instabilities, Hayase *et al*[24].

The proposed scheme is transportive, because only upstream influence is accounted for, conservative and bounded because it fulfills the above criterion and this accounts for the 3 out of the 4 properties stated in the introduction. Its accuracy is demonstrated in the next section.

TEST CASES AND RESULTS

Two linear and one non-linear case have been examined. All cases involve convective dominance, significant stream-grid line skewness and steep gradients of the transported variables. The problems selected are ones for which either analytic solutions or well established numerical results exist, so that the accuracy of the predictions can be judged. Turbulent flow fields are not simulated so that differences from the exact solutions are solely attributed to the properties of the numerical schemes.

a) *Pure convection of a step profile*

This is a simple, yet very stringent, test problem. It involves the pure convection of a step profile by a unidirectional and uniform flow field, which forms an angle θ with the horizontal axis X, *Figure 3a*. The Peclet number is infinite (meaning that physical diffusion is absent). This

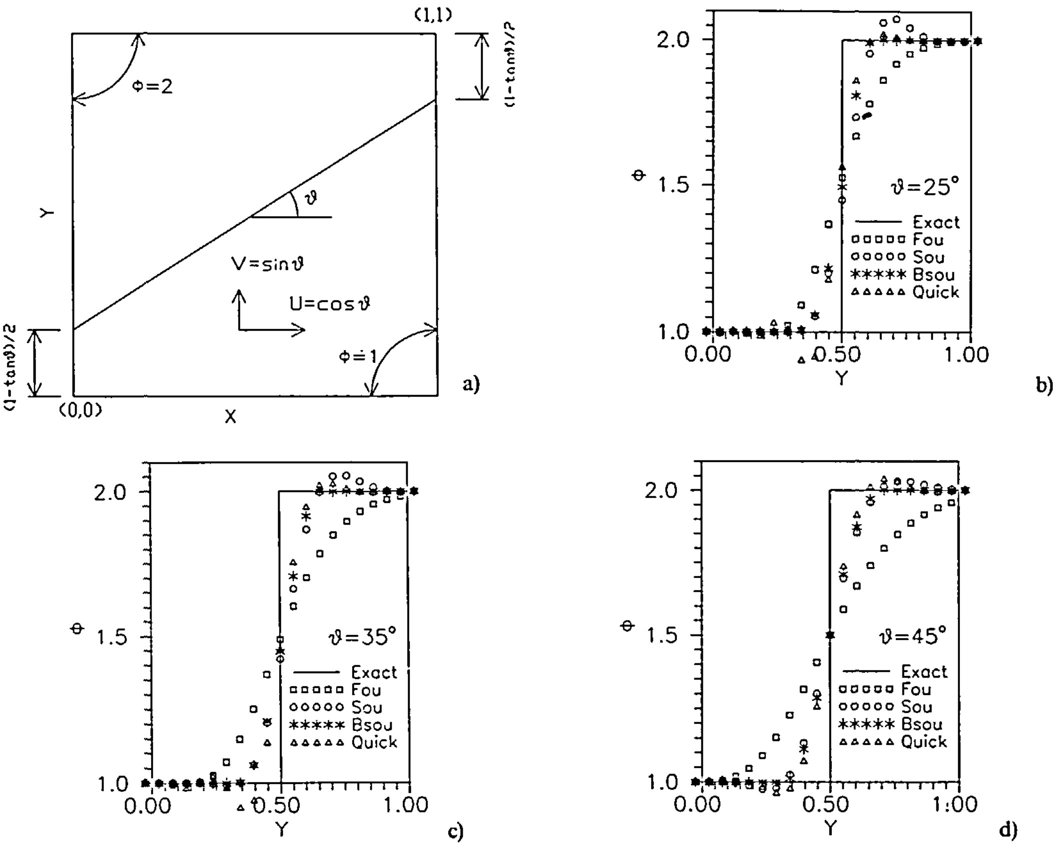


Figure 3 Pure convection of a step profile. (a) Geometry, comparison between *FOU, SOU, BSOU* and the exact solution for flow angles (b) $\theta = 25°$, (c) $\theta = 35°$ and (d) $\theta = 45°$

test problem simulates the case where two parallel streams of equal velocity but unequal temperatures come in contact. The diffusion coefficient of the medium is zero. If the diffusion coefficient were not zero, a mixing layer would form in which the temperature gradually changes from the higher value to the lower one. Since the diffusion coefficient is zero, no mixing layer should form and the temperature discontinuity should persist in the streamwise direction. This means that the formation of a mixing layer is attributed only to the numerical diffusion errors and not to physical diffusion.

Figures 3b, c, d show the performance of *FOU, SOU, BSOU* and *QUICK* by comparing the profile at $X = 0.5$ obtained with each of these schemes against the exact solution, using a uniform 21×21 Cartesian grid for three different angles $\theta = 25$, 35 and 45 deg respectively. As it can be seen *SOU* produces overshoots for all angles and as θ increases, undershoots also appear. *QUICK* produces both overshoots and undershoots for all angles with the undershoots being more exaggerated for smaller angles. The results obtained, using *BSOU*, are free from both overshoots and undershoots while preserving the step resolution of *SOU*. This observation is very important since it indicates that the exact amount of *FOU* is added to *SOU* in order to make the solution wiggle free. *FOU*, although it produces a monotone profile, fails to accurately capture the sharp increase of the step profile leading to a smeared solution which is seen to be most severe at $\theta = 45$ deg.

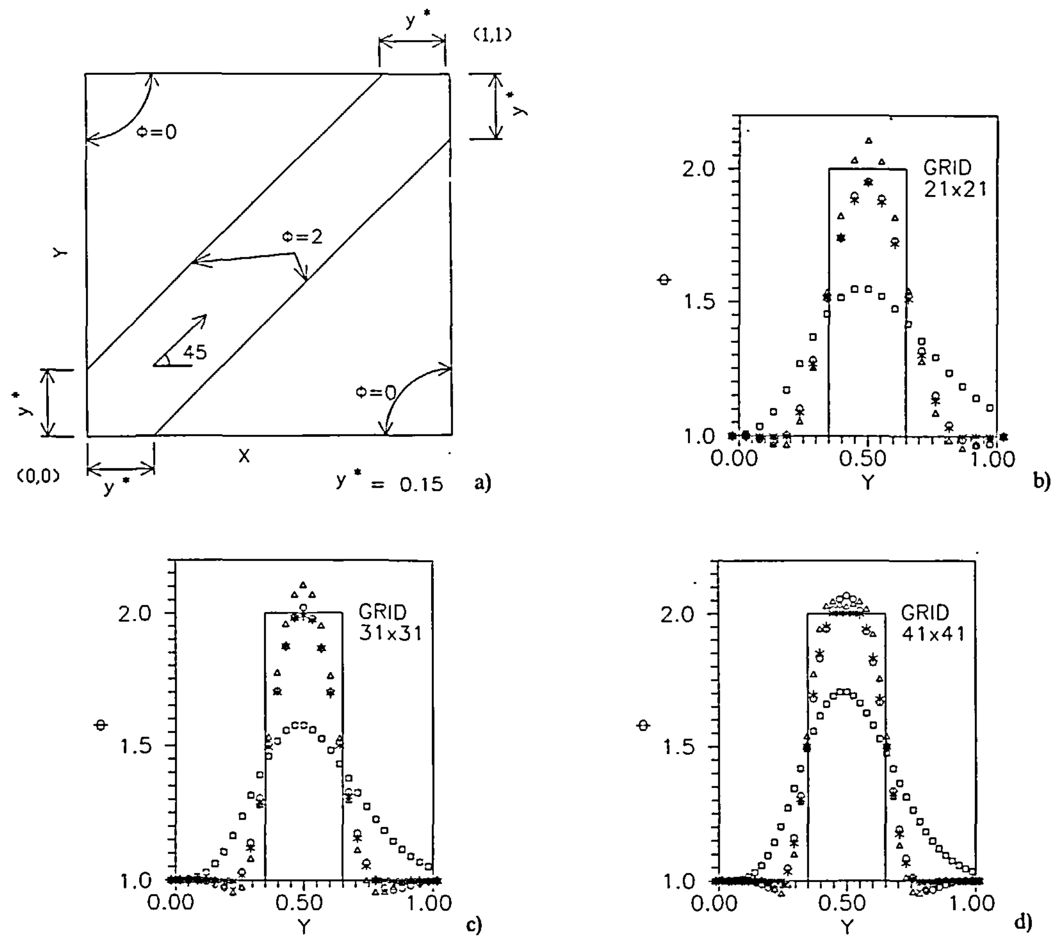


Figure 4 Pure convection of a box profile. (a) Geometry, comparison between *FOU*, *SOU*, *BSOU* and the exact solution for grid sizes (b) 21 × 21, (c) 31 × 31 and (d) 41 × 41. Symbols as in *Figure 3*

b) *Pure convection of a box profile*

This test case was selected in order to investigate the performance of the three schemes in the case where a localized maximum exists in the transported profile and also to check the way that all schemes react to mesh refinement. Again, the Peclet number is infinite. The angle of the flow to the horizontal direction is constant and equal to 45 deg, *Figure 4a*. This test problem simulates, for example, the transport of the turbulence kinetic energy produced in a thin shear layer.

Figures 4b, c, d show the results obtained with the four schemes at $X = 0.5$ for three different computational grids 21 × 21, 31 × 31, 41 × 41 respectively. For all grid sizes *SOU* produces undershoots and for 31 × 31 and 41 × 41 grids also overshoots. *QUICK* always produces both undershoots and overshoots. However, for both *QUICK* and *SOU*, the response to grid refinement is rapid, unlike the response of *FOU*, which even for 41 × 41 grid fails to capture correctly the maximum of the profile. *BSOU* combines the best characteristics of *FOU* and *SOU*, producing a wiggle free solution without creating any physically wrong maxima and minima and at the same time captures the sharp box profile.

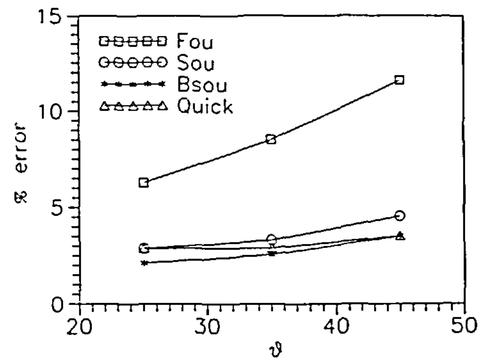


Figure 5 Effect of flow angle θ on the accuracy of *FOU, SOU, BSOU* and *QUICK* schemes (pure convection of a step profile)

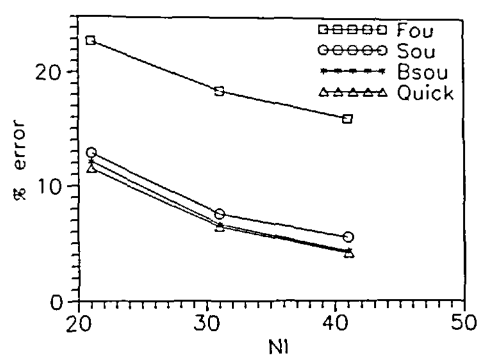


Figure 6 Effect of grid refinement (*NI*) in one direction on the accuracy of *FOU, SOU, BSOU* and *QUICK* schemes (pure convection of a box profile)

For both cases *a*) and *b*), in order to produce the results shown, an under-relaxation factor of 0.8 was employed in order to achieve fully converged solution for the *BSOU* scheme. The explanation for this was given above in the development of the *BSOU* scheme section.

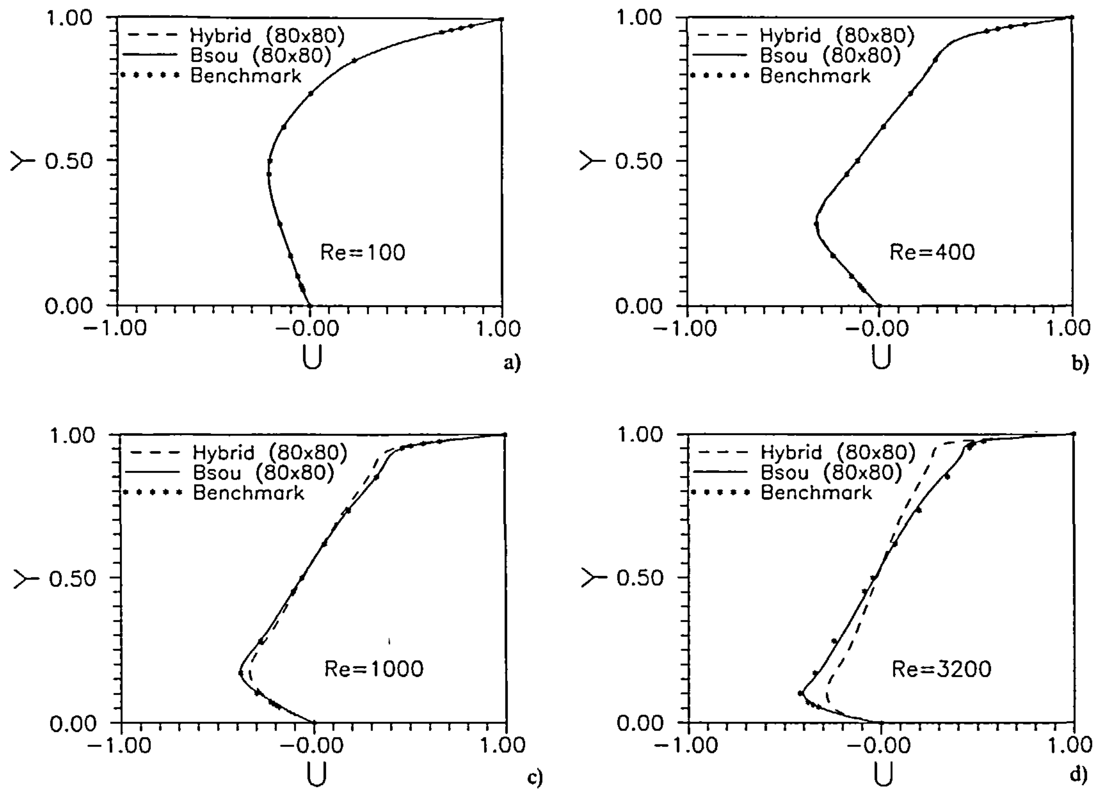
Figures 5 and *6* show the effect of the flow angle θ (convection of a step profile) and grid refinement (convection of a box profile), as expressed by the number of grid points in one direction, on the accuracy of *FOU, SOU, BSOU* and *QUICK* schemes, respectively. Accuracy is estimated by calculating the % error between the exact solution and the numerical results for the Φ distribution at $X = 0.5$. The %error is defined as:

$$\%error = \frac{\sum_{I=2}^{N-1} \left| \frac{\Phi_{exact} - \Phi_{pred.}}{\Phi_{exact}} \right|}{N-2} \times 100 \tag{11}$$

where N is the number of grid points in the Y direction. The points $I = 1, N$ have been excluded since they represent the boundary conditions. Also excluded are points whose Y position coincides with the location of discontinuities since the Φ_{exact} is not defined at these points. Accordingly, in such cases, the denominator of (11) also changes in order to conform to the number of summations in the nominator. From both figures it can be seen that *QUICK* always produces better results than *SOU* which is expected since it has a higher formal order of accuracy than *SOU* (third compared to second order). Also *BSOU* yields in both cases better results than *SOU* which means that the boundedness of the solution increases accuracy. The relative accuracy of *BSOU* and *QUICK* depends on the test case: for the convection of the step profile *BSOU* is more accurate while for the convection of the box profile *QUICK* is more accurate. In all cases the accuracy of *SOU, BSOU* and *QUICK* are comparable, with small differences between their results which are much more accurate than the results of *FOU.*

c) *Flow inside a lid driven cavity*

Having assessed the performance of *BSOU* in linear cases, attention is turned to, practically, more important non-linear ones. The problem considered is that of the recirculating flow inside a lid driven cavity. This is a widely used test problem for checking the accuracy and stability of numerical methods. Five Reynolds numbers were tested (namely, 100, 400, 1000, 3200 and 5000) in order to investigate the performance of *FOU, BSOU* and *QUICK*. For each Reynolds number and scheme 5 runs were made using the following meshes: 20 × 20, 30 × 30, 40 × 40,



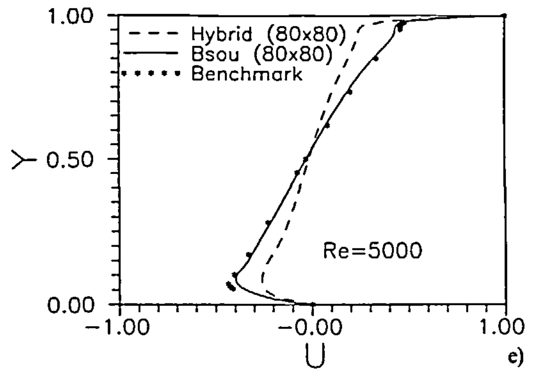


Figure 7 Comparison of the horizontal *U* velocity profiles along the vertical centerline of the cavity obtained with the hybrid and the *BSOU* scheme (80 × 80 mesh) against the benchmark solution for (a) $Re = 100$, (b) $Re = 400$, (c) $Re = 1000$, (d) $Re = 3200$ and (e) $Re = 5000$

60 × 60 and 80 × 80 (totally 75 runs). For all runs the *SIMPLE* algorithm was used and the solutions were assumed converged when all normalized residuals were below 10^{-4}. For almost all runs the underrelaxation factors used were 0.5 for both velocity and pressure, except for the runs with *QUICK* for which 0.3 was used for Reynolds numbers 3200 and 5000. The results obtained using each scheme are tested against the exact solution of Ghia *et al*[25].

Figures 7(a–e) show the horizontal velocity profiles at the geometric centre of the cavity for all Reynolds numbers, obtained with the hybrid and *BSOU* schemes using mesh 80 × 80. For the smaller Reynolds numbers (100, 400) both schemes give very accurate results. As the Reynolds number increases, the accuracy of the hybrid scheme deteriorates; for Reynolds numbers 3200 and 5000 the results compare badly with the exact solution, even with the finest mesh.

Table 1 Strength of the primary vortex

	REYNOLDS NUMBER				
	100	400	1000	3200	5000
HYBRID	0.1032	0.1121	0.1066	0.080	0.0699
BSOU	0.1033	0.1134	0.1165	0.1121	0.1113
Exact	0.1034	0.1139	0.1179	0.1203	0.1189

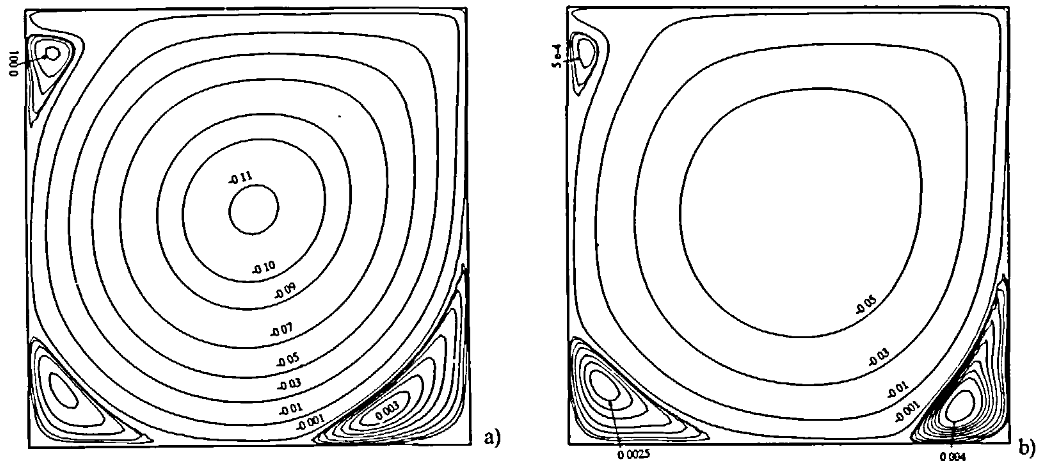


Figure 8 Stream-line pattern of the flow ($Re = 5000$). (a) *BSOU* scheme, (b) Hybrid scheme

The inability of the hybrid scheme, in capturing the variation of the horizontal velocity, has a detrimental effect on the strength of the primary vortex inside the cavity (as expressed by the minimum value of the stream function). *Table 1* compares this strength as predicted using hybrid and *BSOU* (mesh 80 × 80) against the exact solution. It is seen that the strength of the primary vortex is more and more underpredicted by the hybrid scheme as the Reynolds number increases. The results of the *BSOU* scheme are, for all Reynolds numbers, very close to the exact results.

The effect of the discretization schemes on the stream line pattern of the flow is depicted in *Figure 8* (only stream lines for Reynolds 5000 are presented). It is easily seen how numerical diffusion affects the sizes of the recirculation zones. In particular, the vortices in the lower right and the upper left corner have been significantly reduced when the hybrid scheme is used. The effect of diffusion also manifests itself on the pressure distribution inside the cavity, as shown in *Figure 9*. This shows that diffusion not only affects the convected quantities (velocities, temperatures) but the pressure also.

Figure 10 shows the accuracy for hybrid, *BSOU* and *QUICK* for Reynolds numbers 1000 and 3200 versus grid refinement, as expressed by the number of grid points in the horizontal direction of the cavity (the same number of grid points were used for the vertical direction as well). For the hybrid scheme, the convergence towards the exact solution is very slow (a conclusion also been observed in case *b*). On the other hand, the *BSOU* scheme gives markedly better results for all meshes. Compared to *QUICK*, the relative accuracy seems to be case dependent (as already found previously in case *b*). In all cases the results between the two higher order schemes are very close to each other. The same happens also for the rest of the Reynolds numbers.

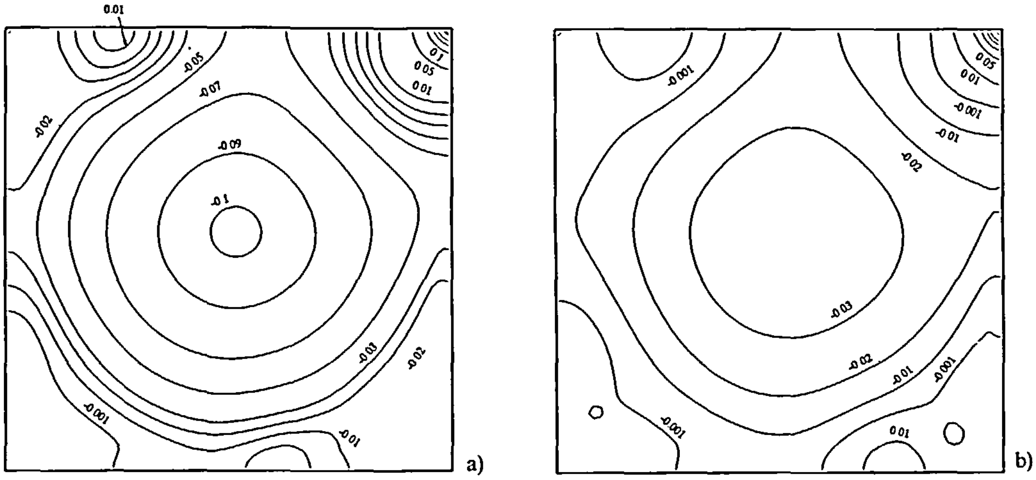


Figure 9 Pressure distribution inside the cavity (Re = 5000). (a) *BSOU* scheme, (b) Hybrid scheme

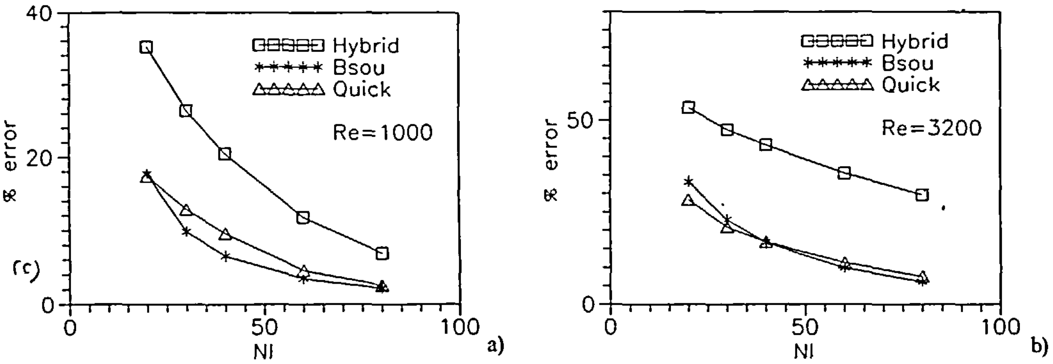


Figure 10 Effect of grid refinement (*NI*) on the accuracy of the solution for hybrid, *BSOU* and *QUICK* schemes. (a) Re = 1000, (b) Re = 3200

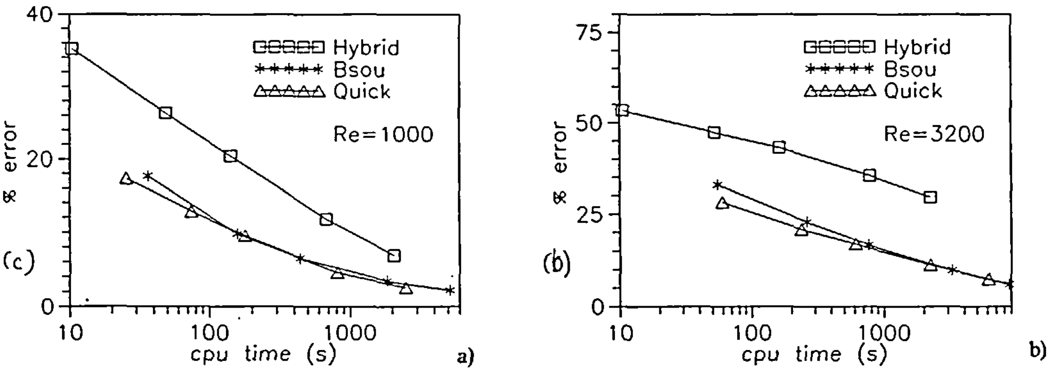


Figure 11 Accuracy versus *CPU* time requirements for hybrid, *BSOU* and *QUICK* schemes. (a) Re = 1000, (b) Re = 3200

Finally, *Figure 11* shows the accuracy against the computational time for the same Reynolds numbers. It is apparent that both *QUICK* and *BSOU* need more computational time than the hybrid scheme. This is not only due to the increased time per iteration, caused by the complexity of the finite difference equation coefficients, but also due to the increased number of iterations, especially for the *BSOU* scheme, caused by the non-linearity of the scheme. The curves for *BSOU* and *QUICK* are very close, giving the same %error for the same computer time, leading eventually to smaller execution times (for the same accuracy) than hybrid. The advantage of *BSOU* over *QUICK* is that it satisfies the boundedness property which enables it to be used for all transport equations as stated in the introduction.

CONCLUSIONS

A flux blending technique between the *FOU* and *SOU* was presented, leading to a boundedness preserving scheme called *BSOU*. The scheme comprises the best characteristics of both schemes and is superior than either. Presently, the scheme is used by the authors for convection terms discretization of all transport equations describing turbulent flow and combustion in a three dimensional, experimental, semi-industrial scale pulverized coal furnace, for which reliable experimental data exist.

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REFERENCES

1 Huang, P. G., Launder, B. E. and Leschziner, M. A. Discretization of non linear convection process: A broad range comparison of four schemes, *Computer Methods in Applied Mechanics and Engineering*, **48**, 1–24 (1985)
2 Leonard, B. P. A stable and accurate convective modelling procedure based on quadratic interpolation, *Computer Methods in Applied Mechanics and Engineering*, **19**, 59–98 (1979)
3 Shyy, W. A study of finite difference approximations to steady state, convection-dominated flow problems, *J. Comp. Physics*, **57**, 415–438 (1985)
4 Castro, I. P. and Jones, J. M. Studies in numerical computations of recirculating flows, *Int. J. Numerical Methods in Fluids*, **7**, 793–823 (1987)
5 Shyy, W., Thakur, S. and Wright, J. Second-order upwind and central difference schemes for recirculating flow computation, *AIAA Journal*, **30**, 923–932 (1992)
6 Vanka, S. P. Second order upwind differencing in a recirculating flow, *AIAA Journal*, **25**, 1435–1441 (1987)
7 Varejao, L. M. C. Flux-spline method for convection-diffusion problems, *Proc. 2nd Congress of Metodos Numericos en Ingenieria*, **2**, 1296–1311 (1993)
8 Gresho, P. M. and Lee, R. L. Don't suppress the wiggles – They are telling you something, *Finite Element Methods for Convection Dominated Flows* (Ed. Hughes, T. J.), ASME Applied Mechs. Dir. Publication AMD34 (1979)
9 McGuirk, J. J., Taylor, A. M. K. P. and Whitelaw, J. H. The assessment of numerical diffusion in upwind difference calculations of turbulent recirculting flows, *Third Int. Symp. on Turbulent Shear Flows*, pp. 206–224 (1981)
10 Benodekar, R. W., Goddard, A. J. H., Gosman, A. D. and Issa, R. I. Numerical prediction of turbulent flow over surface-mounted ribs, *AIAA Journal*, **23**, 359–366 (1985)
11 Gaskell, P. H. and Lau, A. K. C. Curvature-compensated convective transport: SMART, a new boundedness preserving transport algorithm, *Int. J. Numerical Methods in Fluids*, **8**, 617–641 (1988)
12 Leonard, B. P. and Niknafs, H. S. Sharp monotonic resolution of discontinuities without clipping of narrow extrema, *Computers and Fluids*, **19**, 141–154 (1991)
13 Zhu, J. and Leschziner, M. A. A local oscillation-damping algorithm for higher order convection schemes, *Computer Methods in Applied Mechanics and Engineering*, **67**, 355–366 (1988)
14 Peric, M. A finite volume method for the prediction of three-dimensional fluid flow in complex ducts, *PhD thesis, Dept. of Mech. Eng. Imperial College* (1985)
15 Zhu, J. and Rodi, W. Zonal finite-volume computations of incompressible flows, *Computer and Fluids*, **20**, 411–420 (1991)

16 Boris, J. P. and Book, D. L. Flux-Corrected Transport I. *SHASTA*, a fluid transport algorithm that works, *J. Comp. Physics*, **11**, 38–69 (1973)
17 Zalesak, S. T. Fully multidimensional flux-corrected transport algorithms for fluids, *J. Comp. Physics*, **31**, 335–362 (1979)
18 Chapman, M. *FRAM*-Non linear damping algorithsms for the continuity equation, *J. Comp. Physics*, **44**, 84–103 (1981)
19 Sharif, M. A. R. and Busnaina, A. A. Evaluation and Comparison of bounding techniques for convection-diffusion problems, *J. of Fluids Eng.*, **115**, 33–40 (1993)
20 Raithby, G. D. Skew Upstream differencing schemes for problems involving fluids flow, *Computer Meth. in Applied Mech. and Eng.*, **9**, 153–164 (1976)
21 Harten, A. High resolution schemes for hyperbolic conservation laws, *J. Comp. Physics*, **49**, 357–393 (1983)
22 Sweby, P. K. High resolution schemes using flux limiters for hyperbolic conservation laws, *SIAM J. Num. Anal.*, **21**, 995–1011 (1984)
23 Leonard, B. P. The *ULTIMATE* conservative difference scheme applied to unsteady one-dimensional advection, *Comp. Meth. in Applied Mech. and Eng*, **88**, 17–74 (1991)
24 Hayase, T., Humphrey, J. A. C. and Greif, R. A consistently formulated *QUICK* scheme for fast and stable convergence using finite-volume iterative calculation procedures, *J. Comp. Physics*, **98**, 108–118 (1992)
25 Ghia, U., Ghia, K. N. and Shin, C. T. High-Re solutions for incompressible flow using the Navier–Stokes equations and a multigrid method, *J. Comp. Physics*, **48**, 387–411 (1982)