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HIGH ACCURACY MODELING OF ADVECTION AND ADVECTION-DIFFUSION

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SYNOPSIS

Application of unlimited QUICKEST scheme to solve advection and advection–diffusion equations excites overshootings and undershootings in the vicinity of abrupt gradient changes. When universal limiter is utilized to overcome these difficulties, the accuracy is degraded in case of advection-diffusion. The cause of this loss in accuracy is identified and a new strategy is proposed as a remedy. Both linear and nonlinear cases which have analytical solutions are considered to judge the performance of the new strategy. Calculated results show that the modeling of advection-diffusion following the proposed strategy is nonoscillatory and highly accurate.

INTRODUCTION

Heat and mass transfer, pollutant transport, fluid flow and other related processes are mathematically described in terms of differential equations. If the methods of classical mathematics were used for solving these equations, many phenomena of practical interest could not be predicted. Great strides have been made to solve them numerically and sufficient progress has been achieved. But entirely satisfactory numerical method which possesses stability, accuracy, algorithmic simplicity, economy and boundedness (no generation of unphysical spatial oscillation) simultaneously has not yet been developed. Classical numerical methods have wiggles, artificial dispersion, stability and convergence problems depending on particular method, type of flow, and flow condition. Central difference methods are associated with unphysical oscillations and instabilities. First order upwinding often suffers from severe inaccuracy due to numerical diffusion and second order upwinding introduces weak oscillations. Correction of one defect often introduces another equally severe defect (5).

Advection, nonlinearity, multidimensionality and coupling are the major sources of difficulties encountered by numerical methods. Leonard (4) presented a convective modeling procedure based on three points upstream biased interpolation. He developed the QUICK scheme for quasi–steady flow and the QUICKEST scheme for unsteady flow situations. Although both the QUICK and the QUICKEST schemes possess the desirable properties of high accuracy, stability, and algorithmic simplicity, certain fundamental problems remain. When they are applied to purely convective flows of a scalar variable, unphysical overshoots and undershoots are generated in the vicinity of abrupt gradient changes (1, 4, 5, 7). These problems are also encountered when the two schemes are used to model linear advection–diffusion (2). Otherwise, the performance of the QUICKEST scheme is very good for the modeling of linear advection or advection–diffusion.

To get rid of wiggles, Leonard (5) designed ULTIMATE strategy which is applicable to explicit conservative schemes of any order of accuracy. Unphysical oscillations can be also removed by using TVD schemes (3, 9). But all TVD schemes in common use conform to an overly restrictive limiter which tends to make them more diffusive than necessary (10). The accuracy of the usual TVD strategy is limited to essentially second order (8). So ULTIMATE strategy is preferable to TVD schemes.

The application of the ULTIMATE QUICK and QUICKEST schemes successfully alleviate the problems of spurious oscillations for both linear advection (5, 7) and advection-diffusion (2). However, the accuracy is degraded in case of the QUICKEST scheme when applied to advection-diffusion at high Courant number relative to what can be achieved with the unlimited QUICKEST scheme (2).

Since the inherent stability and accuracy of the QUICKEST scheme is superior to that of the QUICK scheme (2, 6), the improvement of the QUICKEST scheme is pursued in this paper. This paper has two objectives. The first one is to identify the actual cause of the loss in accuracy when the universal limiter is applied and to propose a new strategy to avoid the loss. The second objective is to show the performance of the QUICKEST scheme when applied to a nonlinear equation (Burgers equation). The well–known Burgers equation has been chosen because it has analytical solution under certain specific conditions.

BASIS OF THE QUICKEST SCHEME

The QUICKEST scheme uses conservative control volume formulation. The scheme is based on local upstream weighted quadratic interpolation for each interface. It is assumed that the local spatial variation of a field variable is swept downstream by a locally constant advective velocity. Time averaged face value and time averaged gradient are estimated from this convected profile (4). The effect of diffusion on the convected profile is considered in computing the face value (6) and the spatial averages of unsteady term are modeled consistently (4, 5).

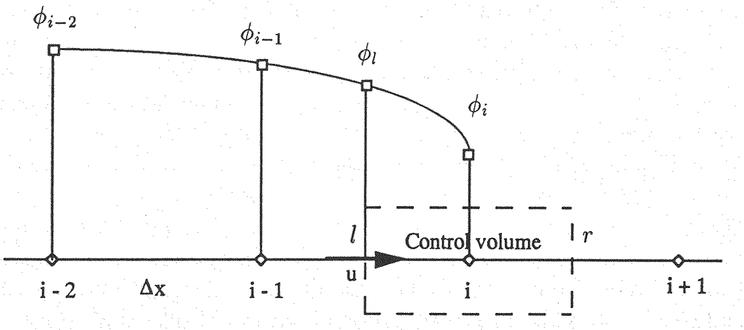

Fig. 1 Quadratic upstream–biased interpolation for left control volume face.

Let us consider unsteady, one dimensional advection-diffusion of a scalar ϕ. This is described by the following differential equation:

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u\phi)}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial \phi}{\partial x}\right) + s \tag{1}$$

where $u(x,t)$ is the advecting velocity; $D(x,t)$ is the diffusion coefficient and $s(\phi, x, t)$ is a source term.

When grid spacing is uniform and the advecting velocity is greater than zero (Fig. 1), the QUICKEST scheme gives, for left face (4, 6),

$$\phi_l = \frac{1}{2}(\phi_i + \phi_{i-1}) - \frac{\gamma_l}{2}(\phi_i - \phi_{i-1}) + \left\{\frac{\alpha_l}{2} - \frac{1}{6}(1-\gamma_l^2)\right\}(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \tag{2}$$

$$\left(\frac{\partial \phi}{\partial x}\right)_l = \frac{\phi_i - \phi_{i-1}}{\Delta x} - \frac{\gamma_l}{2\Delta x}(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \tag{3}$$

where γ_l is the left face Courant number $u_l\Delta t/\Delta x$ and α_l represents the left face diffusion parameter $D_l\Delta t/(\Delta x)^2$.

PRESERVATION OF BOUNDEDNESS

Unphysical oscillations of the QUICKEST scheme is due to its "unlimited form". To overcome these, certain restrictions, so called universal limiter constraints, are applied to control volume face value (ϕ_f) depending on local behavior of ϕ (8).

Fig. 2 shows locally monotonic behavior of ϕ near a control volume face value in a direction normal to the face. In this figure, ϕ_C, ϕ_U and ϕ_D are the central, upstream and downstream node values respectively. In terms of normalized variable, the same information has been depicted in Fig. 3. The normalized variable ($\tilde{\phi}$) is defined as,

$$\tilde{\phi} = \frac{\phi - \phi_U}{\phi_D - \phi_U} \tag{4}$$

For locally monotonic region ($0 \le \tilde{\phi}_C \le 1$), the universal limiter constraints are as follows:

$$\tilde{\phi}_C \le \tilde{\phi}_f \le 1 \qquad for\ \ 0 < \tilde{\phi}_C \le 1 \tag{5}$$

$$\tilde{\phi}_f = 0 \qquad at\ \ \tilde{\phi}_C = 0 \tag{6}$$

$$\tilde{\phi}_f \le \tilde{\phi}_C/\gamma \tag{7}$$

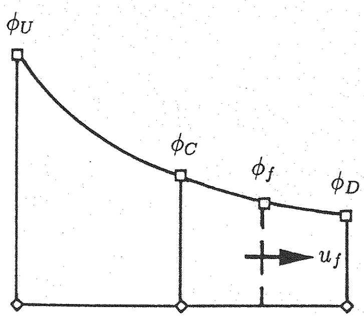

Fig. 2 Locally monotonic behavior across a control volume cell.

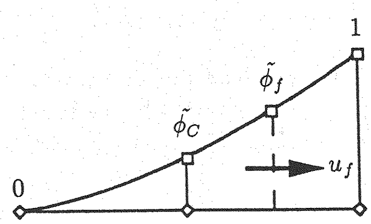

Fig. 3 Locally monotonic behavior in terms of normalized variables.

For non-monotonic range, the universal limiter constraints are given by,

$$\tilde{\phi}_f = \tilde{\phi}_C \qquad for \;\; \tilde{\phi}_C < 0 \quad (8)$$

$$\tilde{\phi}_f = 1 + 0.5(\tilde{\phi}_C - 1) \qquad for \;\; \tilde{\phi}_C > 1 \quad (9)$$

Now the universal limiter constraints can be portrayed in the NVD (Normalized Variable Diagram) as shown in Fig. 4.

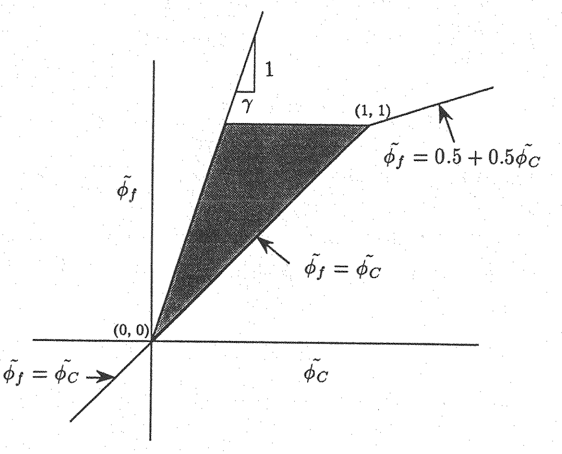

Fig. 4 Universal limiter constraints in normalized variable diagram.

THE CAUSE OF LOSS IN ACCURACY

It has been mentioned earlier that when the universal limiter is applied to obtain bounded results, the QUICKEST scheme shows degradation of accuracy for the modeling of advection-diffusion at high Courant number. This is due to the reason that the control volume face value is then restricted within a narrow region (shaded area in Fig. 4) for locally monotonic behavior of $\tilde{\phi}$. When the Courant number is unity, the control volume face value is devoid of any flexibility, resulting in the highest degradation of the accuracy. For pure scalar convection, the unlimited QUICKEST scheme produces exact results when the Courant number is unity because then point to point transfer over one space step occurs. For locally monotonic ϕ profile, the universal limiter constraints ensure this point to point transfer when the Courant number is unity. It should be noted that the universal limiter constraints were originally developed for the modeling of the linear advective transport equations. So they work very well for linear convective flows.

For advection-diffusion, the universal limiter constraints totally cancel out the contribution of diffusion on the face value when the Courant number is unity and may partially eliminate that effect when the Courant number is less than unity. This cancellation effect may be clearly noticeable only when the Courant number is high enough. What we need is to completely include the effect of diffusion on the control volume face value while maintaining boundedness. Fortunately, this can be achieved by following a very simple strategy which is described in the next section.

THE NEW STRATEGY

The new strategy is to compute the control volume face value in two steps rather than in single step. In the first step, the face value is calculated excluding the effect of diffusion on the convected ϕ profile i.e., ϕ_l is computed from the following equation,

$$\phi_l = \frac{1}{2}(\phi_i + \phi_{i-1}) - \frac{\gamma_l}{2}(\phi_i - \phi_{i-1}) - \frac{1}{6}(1 - \gamma_l^2)(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \qquad (10)$$

Then the universal limiter constraints are applied to this face value and the limited face value, $(\phi_l)_{limited}$ is obtained. In the second step, the effect of diffusion on the convected ϕ profile is added to $(\phi_l)_{limited}$ in order to get the final face value, $(\phi_l)_{final}$, i.e.,

$$(\phi_l)_{final} = (\phi_l)_{limited} + \frac{\alpha_l}{2}(\phi_i - 2\phi_{i-1} + \phi_{i-2}) \qquad (11)$$

The motivation behind this two steps calculation is that universal limiter works well for linear convection, but its performance is not entirely satisfactory for modeling of advection-diffusion. So, if the contribution of diffusion to the control volume face value is separated first to receive universal limiter constraints and then the effect of diffusion on the face value is taken into account, the QUICKEST scheme should work very well. This way of the modeling of diffusion should not pose any difficulty.

When the control volume face value is calculated from Eq. 2 and is not subject to universal limiter constraints, the scheme is hereafter called Unlimited QUICKEST. But if universal limiter constraints are applied to it, the scheme is termed as Limited 1-Step QUICKEST or ULTIMATE QUICKEST. When the proposed new strategy is followed to calculate the control volume face value, the scheme becomes Limited 2-Step QUICKEST. In the absence of diffusion, there is no difference between the Limited 1-Step QUICKEST scheme and the Limited 2-Step QUICKEST scheme and the scheme is then preferably termed as Limited QUICKEST scheme.

TEST CASES

Two problems of scalar advection-diffusion expressed by Eq. 1 and two cases of one dimensional nonlinear Burgers equation were chosen to compare the performance of the variants of the QUICKEST scheme. They are:

(1) Step function of initial concentration (c) distribution described as

$$c(x,0) = \begin{cases} c_0, & x \leq 0 \\ 0, & x > 0 \end{cases} \tag{12}$$

The exact solution of this problem is,

$$c(x,t) = \frac{c_0}{2} erfc\left(\frac{x-ut}{2\sqrt{Dt}}\right) \tag{13}$$

(2) Boundary value problem specified by the following initial and boundary conditions

$$c(x,0) = 0, \qquad 0 < x < \infty \tag{14}$$

$$c(0,t) = c_0, \qquad 0 < t < \infty \tag{15}$$

The exact solution is given by,

$$c(x,t) = \frac{c_0}{2}\left[erfc\left(\frac{x-ut}{2\sqrt{Dt}}\right) + erfc\left(\frac{x+ut}{2\sqrt{Dt}}\right) exp\left(\frac{ux}{D}\right)\right] \tag{16}$$

(3) Wave propagation satisfying the non-viscous 1-D Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 \tag{17}$$

with the following initial distribution of u:

$$u(x,0) = \begin{cases} 1 & (0.5 \geq x) \\ 1.5 - x & (1.5 \geq x > 0.5) \\ 0 & (x > 1.5) \end{cases} \tag{18}$$

The exact solution of this problem is as follows:
For $t < 1.0$,

$$u(x,t) = \begin{cases} 1 & (0.5 + t \geq x) \\ \frac{1.5 - x}{1 - t} & (1.5 \geq x > 0.5 + t) \\ 0 & (x > 1.5) \end{cases} \tag{19}$$

For $t \geq 1.0$,

$$u(x,t) = \begin{cases} 1 & (1 + 0.5t \geq x) \\ 0 & (x > 1 + 0.5t) \end{cases} \tag{20}$$

(4) Propagation of a shock wave satisfying the viscous 1-D Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} \; = \; D\frac{\partial^2 u}{\partial x^2} \tag{21}$$

with the following initial condition:

$$u(x,0) = \begin{cases} u_0 & (x \leq 0) \\ 0 & (x > 0) \end{cases} \tag{22}$$

The analytical solution of this problem is given by,

$$u(x,t) \; = \; u_0 \left[1 + exp\left\{ \frac{u_0}{2D}\left(x - \frac{u_0 t}{2} \right) \right\} \frac{erfc\{-x/(2\sqrt{Dt})\}}{erfc\{(x-u_0 t)/(2\sqrt{Dt})\}} \right]^{-1} \tag{23}$$

RESULTS AND DISCUSSION

Scalar Advection-Diffusion

For problems 1 and 2, all the calculation were performed with the Peclet number of 10. The results of the Unlimited QUICKEST, the Limited 1-Step QUICKEST and the Limited 2-Step

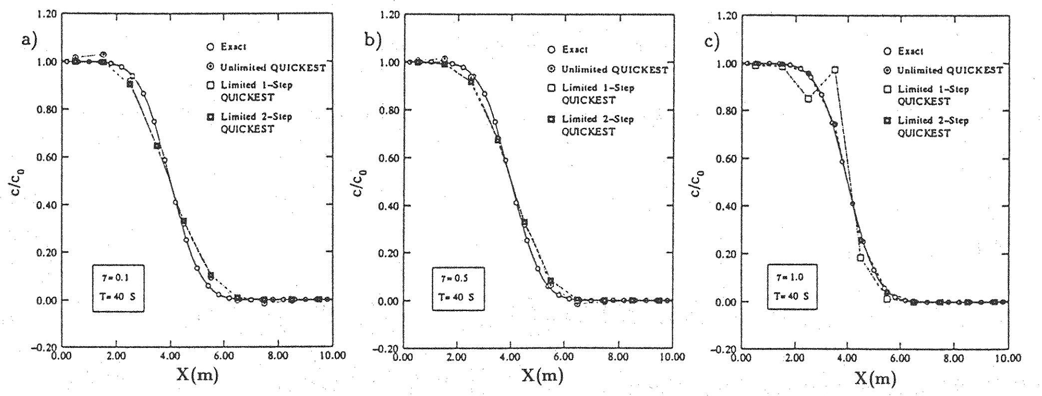

Fig. 5 Results for different Courant number for test case–1.

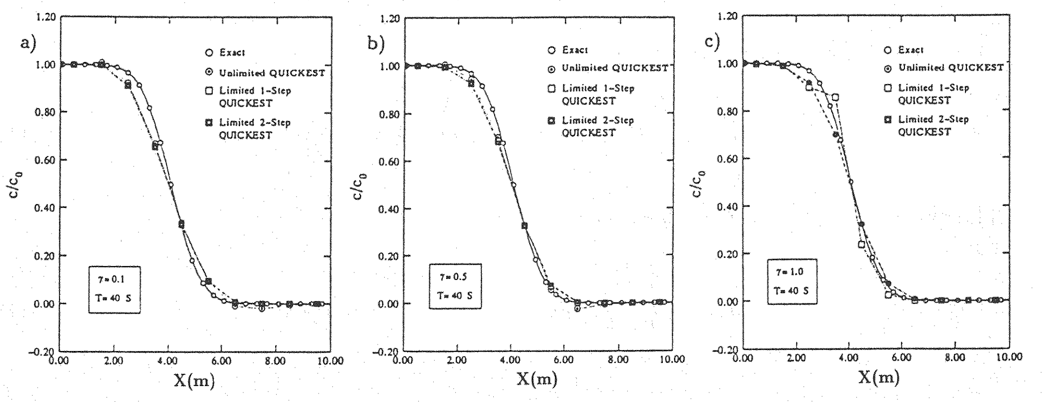

Fig. 6 Results for different Courant number for test case–2.

QUICKEST schemes for different Courant number together with the exact solution for test case 1 are shown in Fig. 5. Fig. 6 compares the results for test case 2. From both figures, it is evident that the Unlimited QUICKEST scheme produces highly accurate nondispersive results, because the scheme is third order accurate in both space and time (6). But the scheme generates small unphysical oscillations near regions of rapid change in gradient (Figs. 5(a), 5(b), 6(a) & 6(b)). The oscillations are reduced as the Courant number is increased (Figs. 5(b) & 6(b)) and completely disappear when the Courant number is unity.

The Limited 1-Step QUICKEST scheme suppresses the unphysical overshoots and undershoots completely when the Courant number is not so high (Figs. 5(a), 5(b), 6(a) & 6(b)). This scheme may not degrade the accuracy of the Unlimited QUICKEST scheme, because the universal limiter constraints have very little chance to interfere with the effect of diffusion on the face value for locally monotonic range. But when the Courant number is unity or close to unity, the Limited 1-Step QUICKEST scheme experiences loss in accuracy (Figs. 5(c) & 6(c)), because the face value has no or little flexibility to correctly capture the effect of diffusion as has been explained in the previous section. The cancellation effect increases as the Courant number approaches to unity and the loss in accuracy is the highest when the Courant number is unity. Not only that, a locally monotonic ϕ profile may become non-monotonic showing spurious peak (Fig. 5(c)) and the results may be highly corrupted (Figs. 5(c) & 6(c)) and therefore, unacceptable.

When the Limited 2-Step QUICKEST scheme is used to overcome the spurious wiggles of the Unlimited QUICKEST scheme, the universal limiter constraints have no chance to interfere with the effect of diffusion on the face value for locally monotonic behavior of ϕ and the results are highly accurate and completely free from unphysical oscillations for all Courant number (Figs. 5 & 6). When the Courant number is small or not so high, the difference between the results of the Limited 1-Step QUICKEST scheme and the Limited 2-Step QUICKEST scheme may be insignificant (Figs. 5(a), 5(b), 6(a) & 6(b)), because then the universal limiter constraints may very slightly change the effect of diffusion as the control volume face value has greater flexibility for locally monotonic range (Fig. 4). For monotonic ϕ profile, the Unlimited QUICKEST scheme and the Limited 2-Step QUICKEST scheme produce the same results (Figs. 5(c) & 6(c)) because then the universal limiter does not modify the control volume face value. So, the Limited 2-Step QUICKEST scheme is the most suitable among the different variants of the QUICKEST scheme for the modeling of linear advection-diffusion.

Burgers Equation

All the calculations were done with $\Delta x = 0.05$ and $\Delta t = 0.025$. For pure advection (Non-viscous Burgers equation), the results of the Unlimited QUICKEST and the Limited QUICKEST schemes at different time, namely 0.5, 1.0, 1.5 and 2.0 are shown in Fig. 7. In this case ther is no difference between the Limited 2-Step QUICKEST scheme and the Limited 1-Step QUICKEST scheme as was notedbefore. The corresponding exact solutions have also been depicted in the same figure. We see that the Unlimited QUICKEST scheme produces appreciable amount of unphysical oscillations behind the wave front. The magnitude of the wiggles increases with time up to 1.0. After that, as the shock advances, the unphysical oscillations may not increase but certainly they do not die out. Except these wiggles, the performance of the Unlimited QUICKEST scheme is satisfactory. When the universal limiter is utilized to get rid of the spurious wiggles, we notice that they do their job very effectively without degrading the accuracy. So, the ULTIMATE strategy is directly applicable for nonlinear advection.

To reveal the performance of the variants of the QUICKEST scheme for nonlinear advection-diffusion (Viscous Burgers equation), a value of 0.01 was given to the diffusion coefficient D. The analytical solution and the numerical results are presented in Fig. 8 at time 0.5 and 2.0. The unlimited scheme simulates the steep wave front very well giving highly accurate results, but the problem is the associated relatively smaller unphysical oscillations behind the wave front. The

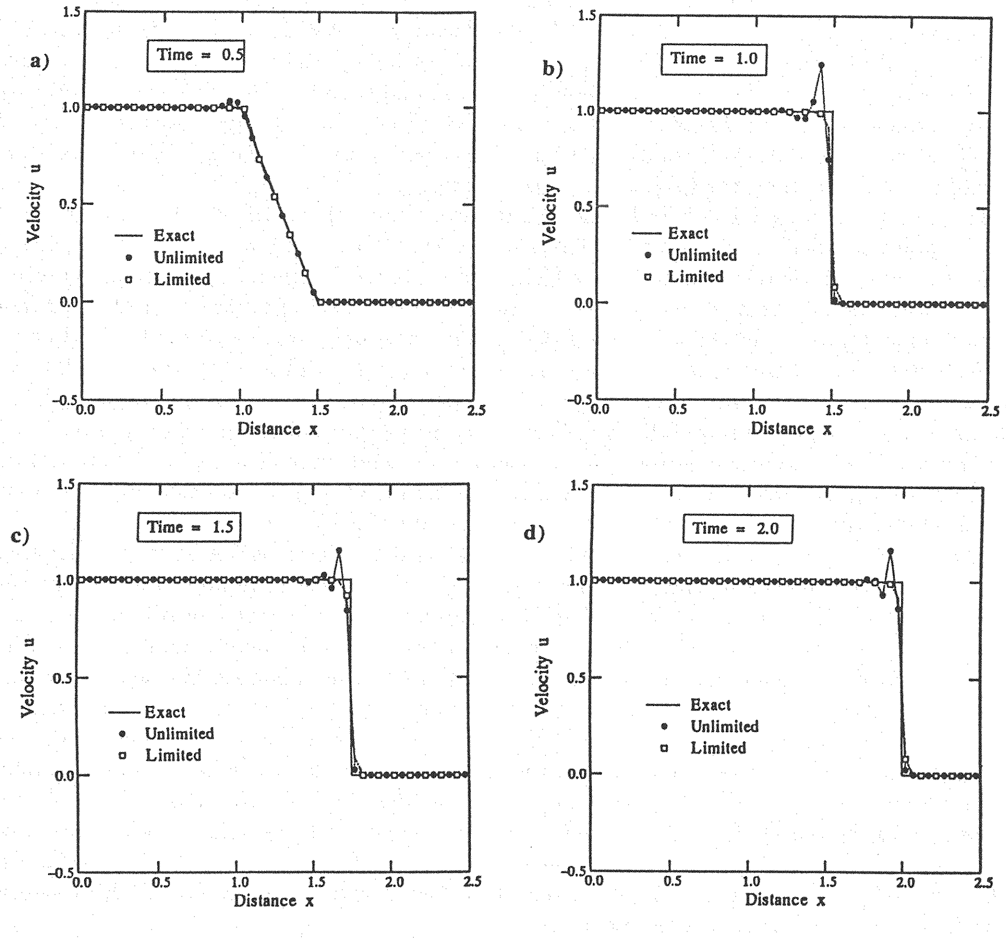

Fig. 7 Results at different time for test case-3.

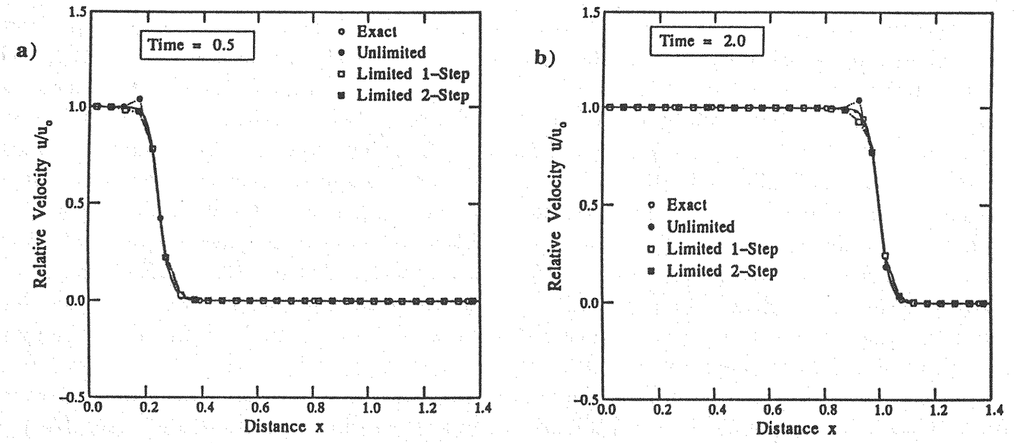

Fig. 8 Results at different time for test case-4.

highest overshooting is just behind the steep front and it decreases very slowly as the time advances. The small undershootings do not disappear with time. Both the Limited 1-Step and 2-Step QUICKEST schemes produce accurate nonoscillatory results, but it is evident from Fig. 8 that the Limited 2-Step scheme captures the wave front better than the Limited 1-Step QUICKEST scheme and hence more accurate. Judging from the results presented in Fig. 8, we can conclude that the universal limiter constraints are also applicable for nonlinear advection-diffusion and the Limited 2-Step scheme is the most suitable among the variants of the QUICKEST scheme for the modeling of nonlinear advection-diffusion.

CONCLUSIONS

This study identifies the actual cause of the loss in accuracy when the ULTIMATE QUICKEST scheme is used for the modeling of advection-diffusion and proposes a new strategy to avoid this. Based on numerical experimentation of both linear and nonlinear cases, the following conclusions can be made:

1. The Unlimited QUICKEST scheme produces highly accurate results, but small overshoots and undershoots are generated near regions of sharp discontinuity in case of scalar advection-diffusion. The unphysical wiggles are much higher for nonlinear advection. Relatively smaller wiggles are produced for nonlinear advection-diffusion.

2. The ULTIMATE strategy is capable of maintaining boundedness for both linear and nonlinear cases. However, the Limited 1-Step QUICKEST (ULTIMATE QUICKEST) scheme shows loss in accuracy in case of advection-diffusion when the Courant number is high.

3. The Limited 2-Step QUICKEST scheme suppresses overshoots and undershoots efficiently while maintaining the high accuracy of the Unlimited QUICKEST scheme for all Courant number. The Limited 2-Step QUICKEST scheme is the most suitable for the modeling of advection-diffusion.

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APPENDIX – NOTATION

The following symbols are used in this paper:

c	=	concentration;
D	=	diffusion coefficient;
s	=	source term;
t	=	time;
u	=	advecting velocity;
x	=	coordinates;
α	=	diffusion parameter;
γ	=	Courant number;
ϕ	=	variable;
ϕ_f	=	values at control volume face;
ϕ_C,ϕ_D,ϕ_U	=	values at central, downstream and upstream node respectively;
$\tilde{\phi}$	=	normalized variable defined by Eq. 4.

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