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Research Article

Computation of LAX Shock Tube Test Case through Large Time Step Scheme with Compressive Limiters

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Abstract: Computation of accurate and efficient numerical results for space vehicle design and analysis is a challenging task because it takes large computational time to predict complex flow physics of space vehicle. Space vehicle travels through continuum as well as rarefied region during flight. Continuum region aerodynamics can be predicted by solving Navier Stokes equation. Explicit schemes require low computational hardware facility but increase computational time by limiting time step to a certain limit defined by stability criteria. An extensive research is being done for last three decades to overcome this stability restriction. Initially, Harten proposed a large time step Total Variation Diminishing (TVD) second order accurate (2K+3) point scheme with explicit formulation under a CFL restriction of K. Harten's developed large time step scheme and its modified Qian's form have been tested with minmod limiter extensively. However detailed analysis of these schemes with more compressive limiter is still in progress. Present research investigates Qian's modified large time step scheme behavior with compressive limiters for complex flow physics. Shock tube problem with Lax boundary condition is computed to point out advantages and short comings of Qian's proposed modified scheme.

Keywords: TVD Scheme, Numerical Dissipation, Shock Tube Problem, LAX.

1. INTRODUCTION

Space vehicles travelling from earth to space takes long time to reach their destination. Particularly missions for outside earth orbit take time in months to get final goal. Computation of their path and flow behavior over them is very costly. In continuum region, Navier-Stokes equation is solved to predict aerodynamics and aero-thermodynamics behavior of space vehicle [1]. Navier-Stocks equations are highly coupled, nonlinear, three dimensional, transient equations. The behavior of these equations is elliptic, parabolic, hyperbolic or mixed characteristics depending upon space vehicle speed, altitude and orientation. Not only Navier-Stocks equations but their simplified form also takes large computational time to predict flow characteristics [2]. Analytical solution of these equations for practical problem is not possible. There are two ways of solving these equations numerically, namely, Explicit formulation or Implicit formulation [3]. Implicit schemes are robust but lack due to excessive hardware and memory requirements for storing and solving large system of discrete equations. Explicit technique [4-5] overwhelms this issue but shortfall due to time step limitation. The stability criteria for an explicit formulation is to limit time stepping [6] which eventually results long computer running times and thus increase computational cost.

Importance of Large Time Step (LTS) Schemes for explicit formulation has been recognized by the researchers and active participation is going on in this field for last three decades. Explicit formulation is easy to setup and code. Flexibility to take large time steps makes explicit formulation matchless with other formulation. Initiate for this task was taken by Harten in 1986 as a consequence of Leveque Randall research in large time step schemes

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for hyperbolic conservation laws [7-9], [5], [10-14]. He presented a second order accurate (2K+3) point Total Variation Diminishing (TVD) scheme with explicit formulation for the computation of weak solutions of hyperbolic conservation laws under a CFL restriction of K [15-17]. Computations for nonlinear wave equation through Harten's large time steps scheme are free of oscillation and precise. However, computation of highly coupled nonlinear system of equations through Harten's large time steps scheme exhibit spurious oscillation in the vicinity of discontinuities.

This nonphysical behavior of Harten's large time step scheme was studied in detailed by Zhan Sen Qian [18-19]. He pointed out that the nonphysical spurious oscillation is due to the inappropriate extension of nonlinear scalar schemes to 1-D nonlinear systems. He recommended that inverse characteristic transformations must be performed by using the local right eigen vector matrix at each cell interface location to get physically valid results and avoid non-physical spurious oscillations. His proposed modification eventually provides oscillation free results.

Harten's large time step scheme and its modified Qian's form have been tested with minmod limiter extensively [9], [13], [20]. Behavior of these schemes with more compressive limiters and complex boundary condition is yet to be reported in the literature and still is a hidden corner. Only reference [21-22] has reported some inside about the behavior of Qian's modified form with centralized MC and super bee limiters. Unfortunately, only SOD boundary condition for shock tube problem was solved in that paper. SOD boundary condition is relatively simple as compared to other boundary conditions used for shock tube problem. Only pressure and density discontinuities are present initially while velocity field is zero at all over the domain in SOD boundary condition. Lax boundary condition for shock tube problem is relatively more complex [23]. Discontinuity in velocity field is also present along with pressure and density discontinuities. Therefore, present study is aimed to investigate Qian's proposed modified large time step scheme behavior in detail for shock tube of Lax boundary condition with compressive limiter. Advantages and short comings of Qian's proposed modified scheme has been pointed out. For thermal analysis and numerical methods [24-27] present the vivid explanation of Navier-Stokes equation for the prediction of aerodynamics and aero-thermodynamics behaviors.

2. NUMERICAL METHOD

The conservation form of 1D Euler equation is given below:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0 \tag{1}$$

$$\frac{\partial \mathbf{U}}{\partial t} + A\frac{\partial \mathbf{U}}{\partial x} = 0 \tag{2}$$

$$\text{where; } U = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix} \quad ; \quad F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho E + p)u \end{bmatrix} \tag{3}$$

$$A = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \begin{bmatrix} 0 & 1 & 0 \\ (\gamma-3)\frac{u^2}{2} & (3-\gamma) & (\gamma-1) \\ (\gamma-1)u^3 - \gamma u E & -\frac{3}{2}(\gamma-1)u^2 + \gamma E & \gamma u \end{bmatrix} \tag{4}$$

equation (1) in numerical flux form can be written as:

$$U_i^{n+1} = U_i^n - \lambda\left(f^n_{i+\frac{1}{2}} - f^n_{i-\frac{1}{2}}\right) \; ; \quad \lambda = \frac{\Delta t}{\Delta x} \tag{5}$$

The numerical flux for Qian's modified LTS TVD is given by:

$$f_{i+\frac{1}{2}} = \frac{1}{2}\,[F_{i+1} + F_i] +$$

$$\left[\frac{1}{2\lambda}\sum_{k=1}^{m} R^k_{i+\frac{1}{2}}\left(g^k_{i+1} + g^k_i\right) - \frac{1}{\lambda}\sum_{l=-K+1}^{K-1}\left\{\sum_{k=1}^{m} R^k_{i+l+\frac{1}{2}}\; C_l\left(v^k + \beta^k\right)_{i+l+\frac{1}{2}}\; \alpha^k_{i+l+\frac{1}{2}}\right\}\right] \tag{6}$$

where m = 3, 4, 5 for one-, two- and three-dimensional problem respectively, and

$$g^k_i = \text{minmod}\left(\tilde{g}^k_{i+\frac{1}{2}}, \tilde{g}^k_{i-\frac{1}{2}}\right) \tag{7}$$

$$\tilde{g}^k_{i+\frac{1}{2}} = \sigma^k_{i+\frac{1}{2}}\alpha^k_{i+\frac{1}{2}} \tag{8}$$

$$\sigma^k_{i+\frac{1}{2}} = \frac{K}{2}\left[\psi\left(\frac{v^k_{i+\frac{1}{2}}}{K}\right)\left\{1 + \frac{K-1}{2}\psi\left(\frac{v^k_{i+\frac{1}{2}}}{K}\right)\right\} - \frac{K+1}{2}\left(\frac{v^k_{i+\frac{1}{2}}}{K}\right)^2\right] \tag{9}$$

$$v^k_{i+\frac{1}{2}} = \lambda\, a^k_{i+\frac{1}{2}} \;; \qquad a = u,\; u + c,\; u - c \tag{10}$$

$$\beta^k_{i+\frac{1}{2}} = \begin{cases} \dfrac{\left(g^k_{i+1} - g^k_i\right)}{\alpha^k_{i+\frac{1}{2}}}, & \text{for} \quad \alpha^k_{i+\frac{1}{2}} \neq 0 \\ 0, & \text{for} \quad \alpha^k_{i+\frac{1}{2}} = 0 \end{cases} \tag{11}$$

$$\alpha^k_{i+\frac{1}{2}} = R^{-1}\Delta_{i+\frac{1}{2}}U \tag{12}$$

$$C_{\pm k}(v) = \begin{cases} c_k\left(\mu_{\mp}(v)\right), & \text{for} \;\; 1 \le k \le K-1 \\ \frac{K}{2}\psi\left(\frac{v}{K}\right), & \text{for} \qquad\quad k = 0 \end{cases} \tag{13}$$

$$\mu_{\pm}(v) = \frac{1}{2}\left[\psi\left(\frac{v}{K}\right) \pm \frac{v}{K}\right] \tag{14}$$

$$R = \begin{bmatrix} 1 & 1 & 1 \\ u & u + c & u - c \\ \frac{u^2}{2} & \frac{u^2}{2} + uc + \frac{c^2}{(\gamma-1)} & \frac{u^2}{2} - uc + \frac{c^2}{(\gamma-1)} \end{bmatrix} \tag{15}$$

$$R^{-1} = \begin{bmatrix} 1 - \frac{(\gamma-1)u^2}{2c^2} & (\gamma-1)\frac{u}{c^2} & -\frac{(\gamma-1)}{c^2} \\ -\frac{u}{2c} + \frac{(\gamma-1)u^2}{4c^2} & \frac{1}{2c} - \frac{(\gamma-1)u}{2c^2} & \frac{(\gamma-1)}{2c^2} \\ \frac{u}{2c} + \frac{(\gamma-1)u^2}{4c^2} & -\frac{1}{2c} - \frac{(\gamma-1)u}{2c^2} & \frac{(\gamma-1)}{2c^2} \end{bmatrix} \tag{16}$$

Mathematical expressions of coefficient of numerical viscosity proposed by Roe, Lax-Wendroff and Harten are given in equations 17 to 20 respectively.

$$\psi(v) = |v| \tag{17}$$

$$\psi(v) = v^2 \tag{18}$$

$$\psi(v) = \begin{cases} \frac{1}{2}\left(\frac{v^2}{\varepsilon} + \varepsilon\right) & |v| < \varepsilon \\ |v| & |v| \geq \varepsilon \end{cases} \quad (19)$$

$$\psi(v) = v^2 + \frac{1}{4} \quad (20)$$

The Table 1 shows the expressions for coefficient functions CI (x) which were obtained after putting different values of K in equation 13.

Table 1. C_l (x) expressions at individual K values

K	C_1	C_2	C_3
2	x^2		
3	x^2 (3-x)	x^3	
4	x^2 (6-4x+x^2)	2x^3 (2-x)	x^4

3. TEST CASE DESCRIPTION

1D shock tube problem test case is widely used for validation purpose of numerical schemes. This test case not only has analytical solution but also has complex flow features. Sod, Lax, Inverse Shock etc. boundary conditions have been specified for shock tube problem by different researchers. Different boundary conditions generate different flow physics which helps researchers to study schemes within intended flow region. Large time step scheme has been examined extensively by means of minmod limiter previously. Present study is aimed to test large time step scheme with compressive limiters explicitly, centralized MC and super bee. 1D shock tube problem with Sod boundary condition has been tested with above mentioned methodology previously. Lax boundary condition is used in current studies. Lax boundary condition is relatively complex as compared to Sod condition due to the presence of velocity discontinuity in initial conditions which is not present in Sod case. Values of pressure, density, and velocity at left and right side of diaphragm for Lax boundary condition is listed in Table 02. The size of computational domain is and the discontinuity is placed at mid of the domain. Number of grid points used in present computations are 1000 and simulations are run for 0.15sec of physical time.

Table 2. Boundary conditions for LAX case

P_R (pa)	ρ_R (kg/m^3)	V_R (m/s)	P_L (pa)	ρ_L (kg/m^3)	V_L (m/s)
0.571	0.5	0.0	3.528	0.445	0.698

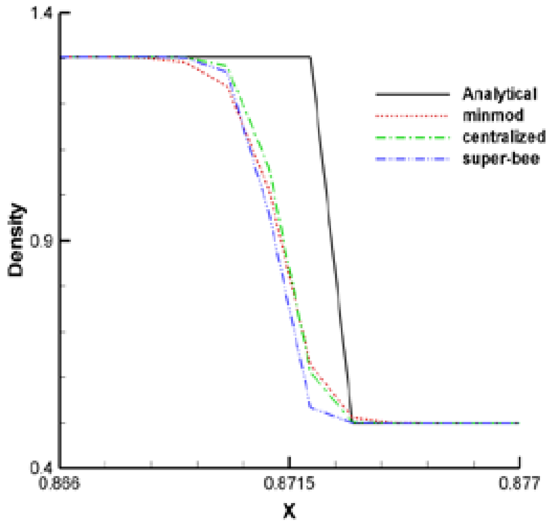
$$U(x,t) = \begin{cases} U_L, \ x < x_o \\ U_R, \ x \geq x_o \end{cases} \quad \text{where, } x_o\text{=0.5} \quad (21)$$

4. RESULTS AND DISCUSSION

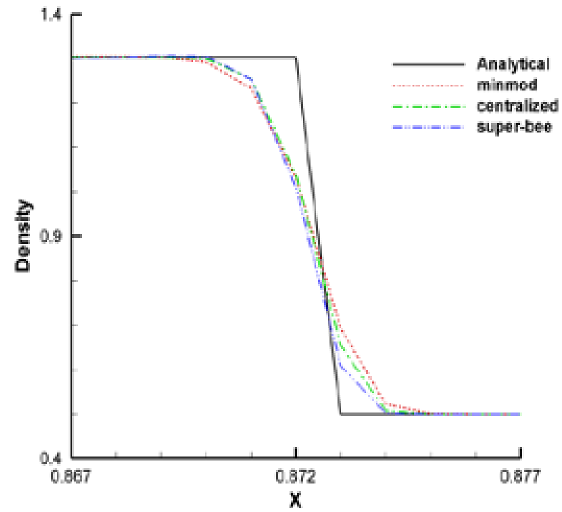
Results of Qian's proposed (2K+3) point explicit formulation large time step total variation diminishing scheme stable under a CFL restriction of K is presented here. Different flux limiters, namely, minmod, centralized MC, and super bee are used for assessment purpose. Attention is paid around expansion, shock, and contact discontinuity regions. Results are analyzed to study stability and accuracy issues related to different limiters with modified large time step scheme. 1D shock tube problem with Lax boundary condition is solved in this comparative study.

Marching in time direction is carried out till 0.15 seconds physical time. This provides expansion fan, shock, and contact discontinuities within computational domain. Value of entropy fix parameter is taken constant (0.1) for all simulations. Comparative study between analytical results and numerical prediction is carried out for LAX case taking K = 1, 2, 3, and 4 for 0.8, 1.8, 2.8, and 3.8 values of CFL, correspondingly.

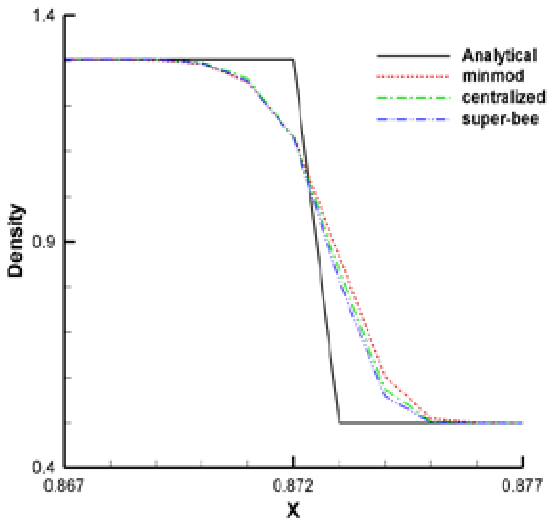
Figure 1 present result near vicinity of shock region. Although all limiters provide oscillation free results however super-bee limiter prediction is less diffusive as compared to other limiters. Figure 2 show results near vicinity of contact region for different CFL values. Results at contact region are identical as at shock region but more dissipative. More dissipation is due to the nature of characteristic lines near contact region. These lines are parallel near contact while convergent near shock. Their convergent nature near shock play vital role to reduce dissipation unlike at contact discontinuity. Figure 3 and Figure 4 present results at start and end of expansion fan respectively. Qualitatively



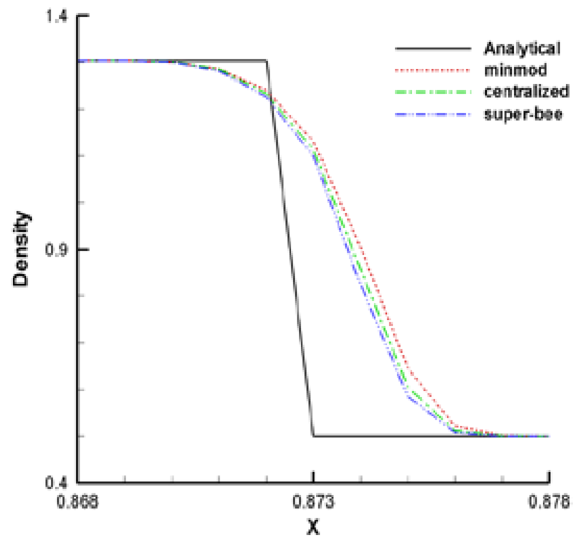
(a) at K=1 & CFL=0.8



(b) at K=2 & CFL=1.8

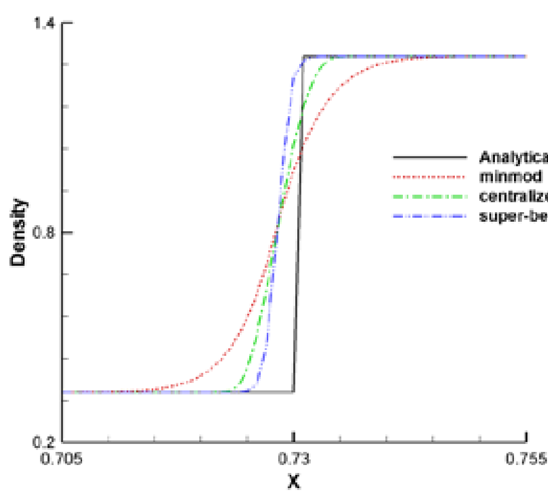


(c) at K=3 & CFL=2.8

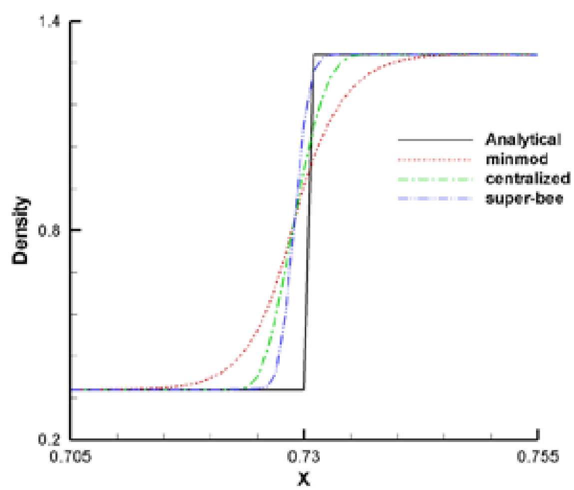


(d) at K=4 & CFL=3.8

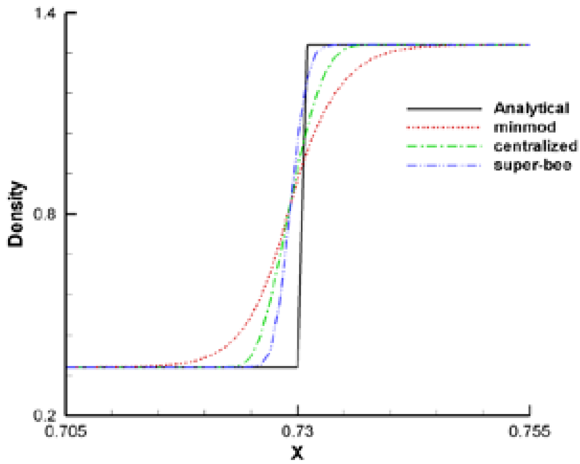
Fig. 1. Near vicinity of Shock



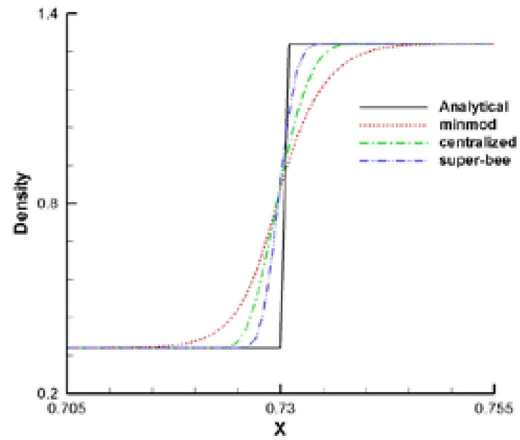
(a) at K=1 & CFL=0.8



(b) at K=2 & CFL=1.8

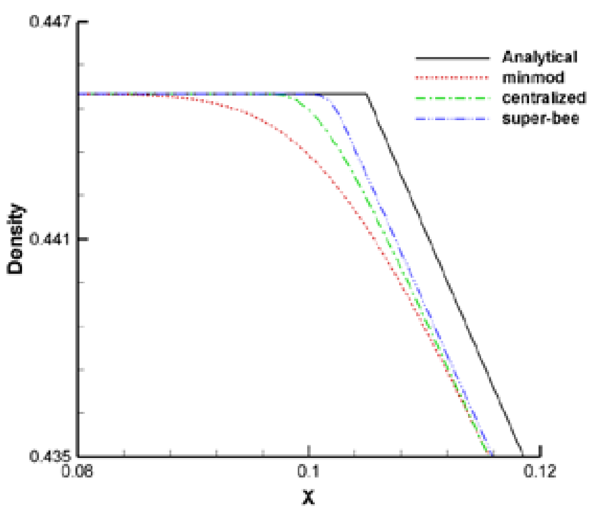


(c) at K=3 & CFL=2.8

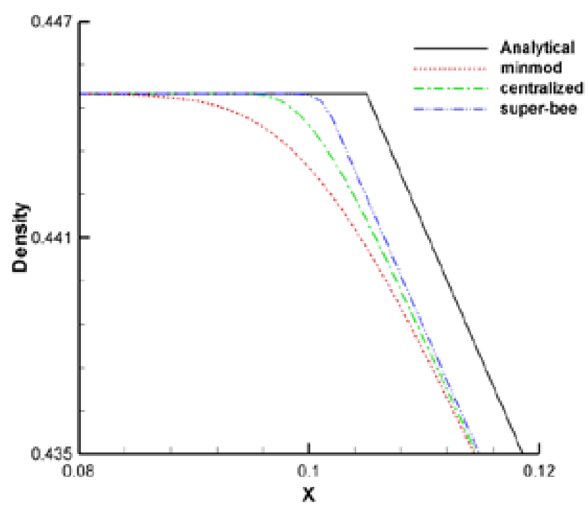


(d) at K=4 & CFL=3.8

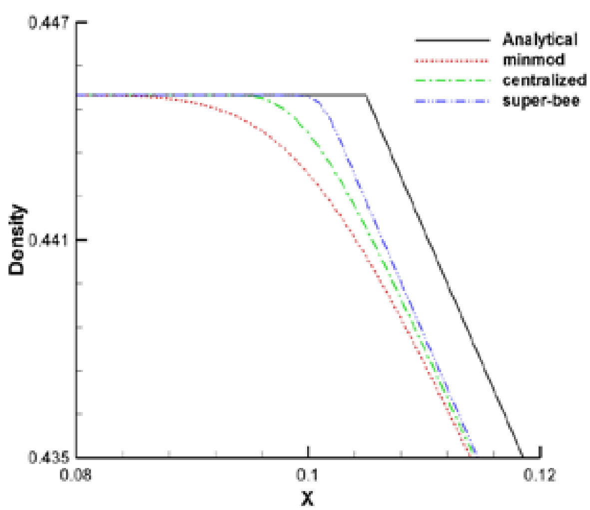
Fig. 2. Near vicinity of Contact



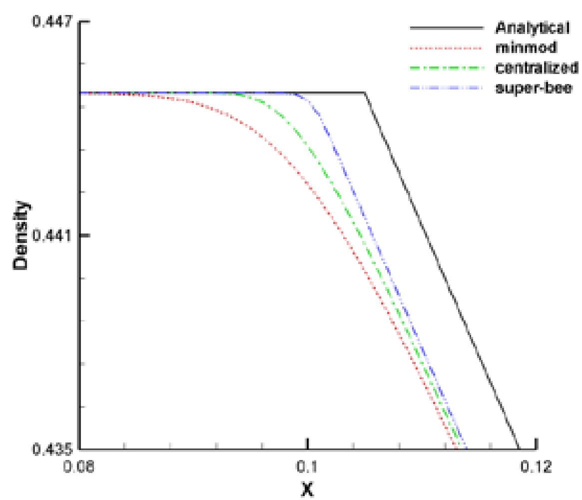
(a) at K=1 & CFL=0.8



(b) at K=2 & CFL=1.8

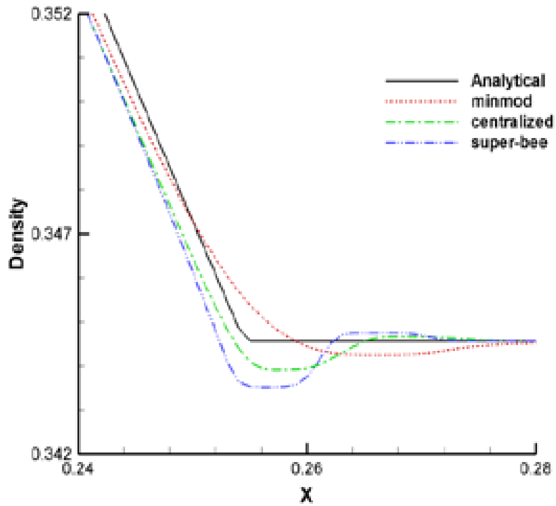


(c) at K=3 & CFL=2.8

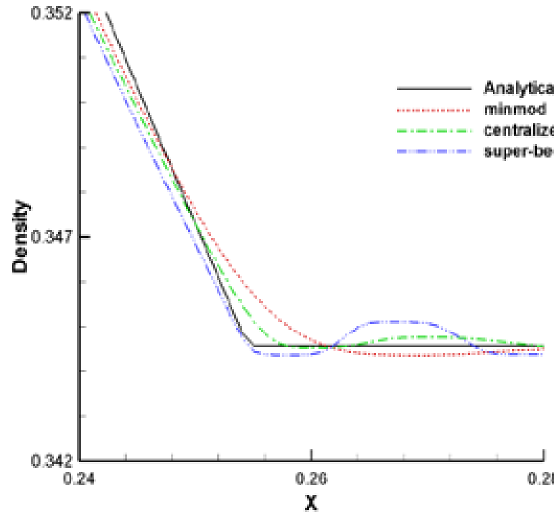


(d) at K=4 & CFL=3.8

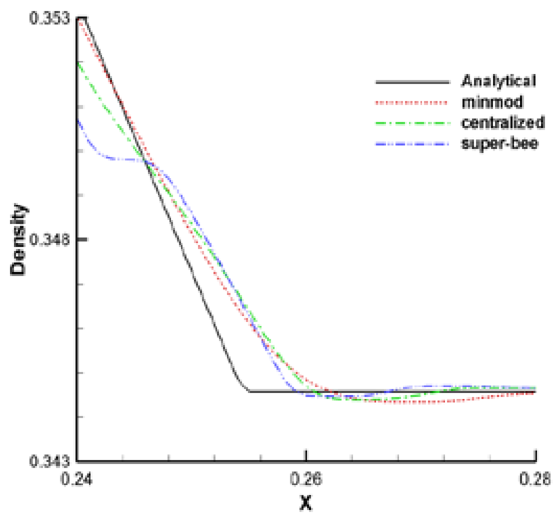
Fig. 3. Near vicinity of Start Expansion



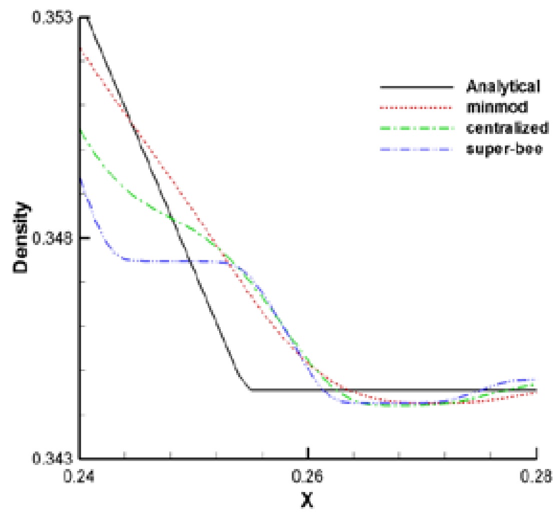
(a) at K=1 & CFL=0.8



(b) at K=2 & CFL=1.8



(c) at K=3 & CFL=2.8



(d) at K=4 & CFL=3.8

Fig. 4. Near vicinity of Expansion End.

expansion fan is predicted well without any non-physical expansion shock. However, deviation with analytical results near start and end of expansion is observed. Despite of minor oscillation at the end of expansion fan, super-bee limiter provides superior results at this region also.

Effect of CFL number is also studied for shock tube problem with Lax boundary condition. For brevity results of super-bee limiter for K = 1, 2, 3, and 4 for 0.8, 1.8, 2.8, and 3.8 values of Courant number, respectively, are presented here. Results near shock are similar to results reported in the past for shock tube problem with Sod boundary condition [10]. For smaller values of CFL number computed shock discontinuity is behind analytical results but travel in forward direction as CFL number increase. Better results are found at contact discontinuity as compared to previously reported results for Sod boundary condition. Present results are smooth and oscillation free while previously reported results for Sod boundary condition have slight oscillations near contact discontinuity. Near expansion fan results are predicted well qualitatively but become more dissipative as CFL number increases. Slight oscillation at the end of expansion fan is noticed which exists too in last reported results.

5. CONCLUSION

Present study is a step to investigate large time step scheme performance with three different compressive limiters (namely minmod, centralized MC, and superbee) to predict complex flow regions. Combination of large time step scheme and compressive limiter is first time investigated to predict shock tube problem with Lax boundary condition. Results are analyzed to study stability and accuracy issues related to different limiters with modified large time step scheme. 1D shock tube problem with Lax boundary condition is solved in this comparative study. Despite minor issue superbee limiter provides efficient and precise results. Results not only qualitatively but quantitatively are very promising and encouraging.

Present study should also be conducted for more complex 2D and 3D test cases to enrich the knowledge and experience related to large time stepping for explicit schemes.

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