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TOTAL VARIATION DIMINISHING FINITE VOLUME SCHEMES FOR ONE DIMENSIONAL ADVECTION-DIFFUSION EQUATION AND THE RELATIONSHIP BETWEEN FLUX LIMITER AND MESH PARAMETERS

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Abstract: Finite volume schemes for one dimensional Advection-Diffusion Equation (ADE) are discussed in this article. As a result, a general explicit difference equation of the form $U_m^{n+1} = aU_{m-1}^n + bU_m^n + cU_{m+1}^n$ is obtained with general coefficients a, b, and c. Stability condition and local truncation error for this general form of explicit difference equation are derived. Then, total Variation Diminishing (TVD) schemes for general flux limiter $\psi(r)$ are also discussed. Further, a relation between flux limiter and mesh length parameters is also obtained. Numerical justification for order of convergence for upwind, central difference and various TVD schemes are also presented.

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1. Introduction

The one dimensional unsteady advection-diffusion problem is given as follows: Find $u(x,t)$ satisfying the governing equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x} \qquad 0 < x < \infty, \quad t > 0, \tag{1}$$

subject to the boundary conditions:

$$u(0,t) = u_0 \qquad t > 0 \tag{2}$$

$$\lim_{x\to\infty} u(x,t) = 0 \qquad t > 0 \tag{3}$$

and initial condition:

$$u(x,0) = 0 \qquad 0 < x < \infty, \tag{4}$$

where, u is the property being transported; v the prescribed transport velocity; and D the diffusion coefficient.

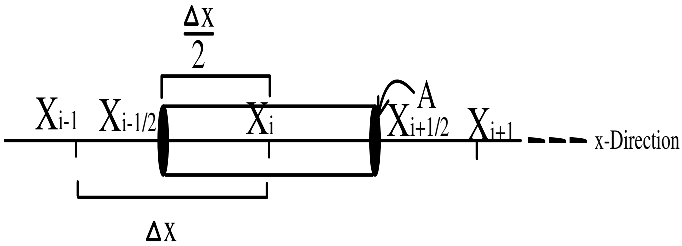
The above advection-diffusion equation (ADE) is used to model the transportation of chemical species beneath the earth surface. Such type of ADE arises in atmospheric pollution caused by smoke, pollution of groundwater and other environmental pollution problems. The diffusion of tracers, spread of chemical solutes and contaminant discharge in porous media, the sea water intrusion and thermal pollution of river systems can also be modeled by above mentioned equation. The raising demand in environmental issues motivate researchers to study about advection-diffusion equation. Solution to ADE will help to tackle challenges in many environmental issues. Therefore, theoretical and numerical studies about ADE are very important.

The solution to above ADE equation is derived in many articles in the literature. Analytical solution and numerical solution by finite difference and finite element techniques are presented in the research articles for the past four decades. van Genuchten [19] is one of the pioneers who investigated solution to advection diffusion equation using transform technique. In general, analytical solution to advection-diffusion type equation is mainly based on Laplace, Fourier and other integral transform techniques. The work done by Yates [21] and Hunt [12] on one dimensional species transport in porous medium problems are the noteworthy contributions to analytical solution methods. These transform techniques are discussed in semi-infinite or infinite domain. Therefore, it leads to appearance of the error function or an exponential function or an infinite series in its solution, which cannot be evaluated exactly. Instead of truncating the closed form solution, numerical method can be a desirable alternate for good approximate solution which is also more appropriate for the practically collected data set.

The numerical solution to ADE initially started with finite difference approximation which is well established at present. In the recent years, Halil Karahan [11] discussed explicit and implicit finite difference methods with the help of spreadsheets. Abolfazl Mohammadi *et. al.* [1] and Mehdi Dehghan [15] presented weighted average technique to solve advection-diffusion equation. The next endeavor in the numerical methods for ADE is the finite element method. In 1988, Frind [10] used a finite element method (FEM) for advection-diffusion equation with free exit boundary. Fruther, Daus *et. al.* [6] made a comparative study in finite element formulation of ADE with finite difference methods. Then, the comparison between mesh-free radial basis function method and mesh-dependent finite difference methods for linear advection diffusion equation was established by Boztosun and Charafi [3]. Siegel *et. al.* [17] and Anis Younes [2] developed the discontinuous Galerkin method to find solution to ADE. A few other FEM methods are also discussed and analyzed by researchers. For example, Nguyen and Reynew [16] applied space-time least-square finite element method. Jim Douglas Jr *et. al.* [13] presented modified method of characteristics. A time-splitting technique for the advection-diffusion equation in groundwater is discussed by Mazzia *et. al.* [14].

Finite volume method (FVM), a modern numerical technique in which mass conservation principle is preserved locally, become popular in recent years. The other advantages of FVM are treatment to flux boundary conditions and easy implementation mesh free techniques. Godlewski *et. al.* [8], Eymard *et. al.* [7] LeVeque [9]made a big contribution in the development of finite volume method. The affiliation of total variation diminishing technique to FVM strengthen the numerical computation. Further, the introduction of flux limiters in TVD scheme adds more meaning to practical problems, because it controls the numerical diffusion. Bram van Leer [4] has introduced the limiter in his paper in 1974. Thereafter, researchers like van Albada , Sweby, Roe, Chatkravathy and Osher are contributed to the development of various flux limiters and deriving TVD region.

The total variation diminishing finite volume methods for advection diffusion equation with flux limiter are discussed in this paper. Further, a detailed analysis on stability, consistency and order of convergence for the central difference, upwind and TVD schemes are also discussed. The relation between flux limiter and mesh parameters is established in this article.



Analytical solution to species transport equation

$$R\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} = -ku \qquad 0 < x < \infty, \quad t > 0 \tag{5}$$

with conditions (2), (3) and (4) is given by (See,[5]):

$$\begin{aligned} u(x,t) &= \frac{u_0}{2} exp\left(\frac{vx}{2D}\right)\left[exp\left(-\frac{mx}{2D}\right) erfc\left(\frac{Rx - mt}{\sqrt{4DRt}}\right)\right. \\ &+ \left. exp\left(\frac{mx}{2D}\right) erfc\left(\frac{Rx + mt}{\sqrt{4DRt}}\right)\right], \end{aligned} \tag{6}$$

where $m = \sqrt{v^2 + 4kD}$. Solution to advection-diffusion equation (1) is obtained by putting $k = 0$ and $R = 1$ in above.

2. Mathematical Description

In this section, a finite volume formulation is presented for the advection-diffusion equation (1) mentioned in previous section. The vector form of (1) is given by

$$\frac{\partial u}{\partial t} = \overline{\nabla}.(\overline{\nabla} Du) - \overline{v}.\overline{\nabla}(u). \tag{7}$$

The computational domain is discretizied by non overlapping control volumes. Following control volume (CV) is considered for the numerical schemes: Here, the y and z dimensions are infinitesimal. Therefore, $\Delta V = \Delta x$. where Δx is the spatial discretization length. Further, $m+1, m, m-1$ are nodal indices and $m - \frac{1}{2}$ and $m + \frac{1}{2}$ are face indices of control volume.

The governing equation is integrated over the control volume locally. The volume integral is then converted to a integral over a boundary surface by applying Gauss divergence theorem. Further, a suitable numerical approximation is used for advection and diffusion terms at the boundary surface. The central difference scheme is applied for both advection and diffusion terms (See, [20]). Let Δt be be a small increment in time t. Integrating above over the control volume in the time interval $(t, t+\triangle t)$, we obtain

$$\begin{aligned}\int_t^{t+\Delta t}\int_{CV}\frac{\partial u}{\partial t}dV\,dt &= \int_t^{t+\Delta t}\int_{CV}\overline{\nabla}.(\overline{\nabla}Du)dV\,dt \\ &- \int_t^{t+\Delta t}\int_{CV}\overline{v}.\overline{\nabla}(u)dV\,dt.\end{aligned}$$

Applying Gauss divergence theorem, we have that

$$\begin{aligned}\int_{CV}(u^{n+1}-u^n)dV &= \int_t^{t+\Delta t}\int_S \overrightarrow{n}.\overline{\nabla}(Du)dS dt \\ &- \int_t^{t+\Delta t}\int_S \overrightarrow{n}.(u\overline{v})dS dt\end{aligned}$$

where $\overrightarrow{n}$ is the unit normal to the surface S. One dimensional formulation of above integral leads to

$$\begin{aligned}(U_m^{n+1}-U_m^n)\Delta x &= D\left[\left(\frac{\partial u}{\partial x}\right)^n_{m+\frac{1}{2}} - \left(\frac{\partial u}{\partial x}\right)^n_{m-\frac{1}{2}}\right]\Delta t \\ &- v[u^n_{m+\frac{1}{2}} - u^n_{m-\frac{1}{2}}]\Delta t.\end{aligned}$$

where U_m^n be the approximation of $u(x,t)$ at the nodal point (x_m, t_n). Here D and v are assumed to be constants. Using the central difference approximation for the derivative term, we obtain

$$(U_m^{n+1}-U_m^n)\Delta x = \frac{D\Delta t}{\Delta x}[U^n_{m-1} - 2U^n_m + U^n_{m+1}] - v[u^n_{m+\frac{1}{2}} - u^n_{m-\frac{1}{2}}]\Delta t. \quad (8)$$

Let us discuss different numerical schemes according to suitable approximation for the advection term namely, the central difference, upwind and TVD schemes.

Central Difference Scheme: Use the following linear interpolation to advection term at the cell faces

$$u^n_{m+\frac{1}{2}} = \frac{U^n_{m+1}+U^n_m}{2} \qquad\qquad u^n_{m-\frac{1}{2}} = \frac{U^n_m+U^n_{m-1}}{2}, \quad (9)$$

to obtain the first numerical scheme from (8)

$$U_m^{n+1} = \left[\frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{2\Delta x}\right] U_{m-1}^n + \left[1 - \frac{2D\Delta t}{\Delta x^2}\right] U_m^n + \left[\frac{D\Delta t}{\Delta x^2} - \frac{v\Delta t}{2\Delta x}\right] U_{m+1}^n. \quad (10)$$

Upwind Scheme: The upwind scheme in a positive direction ($v > 0$) is given by the following approximation to advection term in (8),

$$u_{m+\frac{1}{2}}^n = U_m^n \qquad u_{m-\frac{1}{2}}^n = U_{m-1}^n. \quad (11)$$

The second numerical scheme is given by

$$U_m^{n+1} = \left[\frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x}\right] U_{m-1}^n + \left[1 - \frac{2D\Delta t}{\Delta x^2} - \frac{v\Delta t}{\Delta x}\right] U_m^n + \left[\frac{D\Delta t}{\Delta x^2}\right] U_{m+1}^n. \quad (12)$$

Total Variation Diminishing Scheme: It is possible to get higher order total variation diminishing schemes by reconstructing advection term $u_{m+\frac{1}{2}}$ and $u_{m-\frac{1}{2}}$ in equation (8) with anti-diffusion term. The anti-diffusion term controls the numerical diffusion which is explained in truncation error for TVD scheme in section 4. Expanding $u_{m+\frac{1}{2}}$ in Taylor's series and truncating after second term, we have

$$u_{m+\frac{1}{2}} \approx u_m + \frac{\Delta x}{2}(\frac{\partial u}{\partial x})_m.$$

The flux term $(\frac{\partial u}{\partial x})$ in above is called the anti-diffusion term. Introducing flux limiter $\psi(r)$ to control anti-diffusion and using forward difference approximation for flux term, we obtain

$$u_{m+\frac{1}{2}} \approx u_m + \frac{\psi(r_m)}{2}(u_{m+1} - u_m)$$

where $r_m = \dfrac{u_m - u_{m-1}}{u_{m+1} - u_m}$. Therefore,

$$u_{m+\frac{1}{2}} \approx u_m + \frac{\psi(r_m)}{2}(u_{m+1} - u_m)$$

and

$$u_{m-\frac{1}{2}} \approx u_{m-1} + \frac{\psi(r_{m-1})}{2}(u_m - u_{m-1}).$$

Using $u_{m+\frac{1}{2}}$ and $u_{m-\frac{1}{2}}$ in equation (8), we obtain

$$U_m^{n+1} = \left[\frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x} - \frac{v\Delta t}{2\Delta x}\psi(r_{m-1})\right] U_{m-1}^n$$

$$
\begin{aligned}
&+ \left[1 - \frac{2D\Delta t}{\Delta x^2} - \frac{v\Delta t}{\Delta x} + \frac{v\Delta t}{2\Delta x}[\psi(r_{m-1}) + \psi(r_m)]\right] U_m^n \\
&+ \left[\frac{D\Delta t}{\Delta x^2} - \frac{v\Delta t}{2\Delta x}\psi(r_m)\right] U_{m+1}^n. \qquad (13)
\end{aligned}
$$

3. Stability

In this section, we shall discuss the stability of general form of the explicit difference scheme and hence for central, upwind, and TVD scheme as particular cases. From (10), (12) and (13), the general form of explicit scheme may be written as

$$U_m^{n+1} = aU_{m-1}^n + bU_m^n + cU_{m+1}^n, \qquad (14)$$

where a, b, c are appropriate coefficients for the relevant scheme.

Definition 1. A scheme $U_m^{n+1} = G(U_{m-k}^n, ..., U_m^n, ...U_{m+p}^n)$ is said to be monotone scheme if G is non-decreasing function of each of its argument. So, $\frac{\partial G}{\partial u_i}(U_{-k}, ..., U_0, ...U_p) \geq 0, i = -k, ..., p$.

Theorem 2. *Let $U_m^{n+1} = aU_{m-1}^n + bU_m^n + cU_{m+1}^n$ be the general form explicit finite difference scheme for the linear time-dependent partial differential equation. If $a \geq 0,\ b \geq 0$, and $c \geq 0$ with $a + b + c = 1$, then the scheme is stable and monotone.*

Proof. Let $U_m^{n+1} = aU_{m-1}^n + bU_m^n + cU_{m+1}^n$ be the general form of explicit finite difference numerical scheme. Let $U_m^n = B\xi^n e^{im\theta}$. The von Neumann stability analysis for the above difference scheme implies,

$$\xi = ae^{-i\theta} + b + ce^{i\theta} = b + (a + c)(\cos\theta) + i(c - a)\sin\theta.$$

The amplification factor $'\xi'$ should meet the condition $|\xi| \leq 1$ in order the numerical scheme (14) to have a stable solution which is equivalently $|\xi|^2 \leq 1$ (Smith, [18]).We therefore have that,

$$
\begin{aligned}
b^2 + (a + c)^2\cos^2\theta + 2b(a + c)\cos\theta + (c - a)^2\sin^2\theta &\leq 1 \\
\Leftrightarrow a^2 + b^2 + c^2 + 2ac(\cos^2\theta - \sin^2\theta) + 2b(a + c)\cos\theta &\leq 1 \\
\Leftrightarrow (a + b + c)^2 - 2b(a + c)(1 - \cos\theta) - 2ac(1 - \cos 2\theta) &\leq 1 \\
\Leftrightarrow (a + b + c)^2 \leq 1 + 4b(a + c)\sin^2\frac{\theta}{2} + 4ac\sin^2\theta & \\
\Leftrightarrow (a + b + c)^2 \leq 1 + 4b(a + c)\sin^2\frac{\theta}{2} + 16ac\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2} &
\end{aligned}
$$

$$\Leftrightarrow (a+b+c)^2 + 16ac\sin^4\frac{\theta}{2} \leq 1 + 4b(a+c)\sin^2\frac{\theta}{2} + 16ac\sin^2\frac{\theta}{2}.$$

Maximizing the trigonometric functions in above inequality with respect to their argument θ, we obtain

$$(a+b+c)^2 \leq 1 + 4b(a+c). \tag{15}$$

Let us assume that $a \geq 0, b \geq 0, c \geq 0$ and $a+b+c = 1$. Then the condition (15) is satisfied. Therefore, the scheme (14) is stable. Let $G(U^n_{m-1}, U^n_m, U^n_{m+1}) = aU^n_{m-1} + bU^n_m + cU^n_{m+1}$ be the function. From (14), $U^{n+1}_m = G(U^n_{m-1}, U^n_m, U^n_{m+1})$. By definition (1) $\frac{\partial G}{\partial u_i}(U_{-1}, U_0, U_1) \geq 0, i = -1, 0, 1$,which implies that the scheme is monotone. □

Remark 3.1. The monotonicity guarantees that the solution obtained from explicit finite difference scheme will not oscillate.

We shall discuss below the stability of central difference, upwind and TVD scheme as a particular case of general explicit scheme.

Stability Condition for Central Difference Scheme: From equation (10), we have

$$a = \frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{2\Delta x} \qquad b = 1 - \frac{2D\Delta t}{\Delta x^2} \qquad c = \frac{D\Delta t}{\Delta x^2} - \frac{v\Delta t}{2\Delta x}$$

$$a+b+c = 1 \qquad 4b(a+c) = -\frac{16D^2\Delta t^2}{\Delta x^4} + \frac{8D\Delta t}{\Delta x^2}$$

stability condition (15) implies

$$\frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}. \tag{16}$$

The above condition is nothing but the CFL condition for pure diffusion. It should be noted that the above stability condition is independent of velocity term v. Therefore, the stability behavior of central difference scheme can not be judged for pure advection case.

It is already assumed that the coefficients of explicit schemes are positive. The negative coefficients may produce oscillations in numerical solution. The positivity (or monotonicity) of solution is very essential. Therefore, the coefficient c must be greater than or equal to zero ($c \geq 0$) in order to obtain monotone solution, which is eventually

$$\frac{D}{\Delta x} - \frac{v}{2} \geq 0.$$

$$ie, \frac{v\Delta x}{D} \leq 2. \tag{17}$$

The left side quantity in above is the famous Peclet Number, which means that the central difference scheme is valid for Peclet number less than or equal to 2. In other words, the central difference scheme is suitable for diffusion dominated flow only. Alternatively, the discretization length Δx can made be very small (eventually Δt also) for advection dominated problems. Therefore, the conditions (16) and (17) are essential for the stability of central difference scheme.

Stability Condition for Upwind Scheme: In this case, from (12)

$$a = \frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x} \qquad b = 1 - \frac{2D\Delta t}{\Delta x^2} - \frac{v\Delta t}{\Delta x} \qquad c = \frac{D\Delta t}{\Delta x^2}$$

using the above values of a, b, c in the stability condition (15), we obtain

$$\Delta t \leq \frac{(2D + v\Delta x)\Delta x^2}{4D^2 + 4Dv\Delta x + v^2\Delta x^2}. \tag{18}$$

The above equation satisfies the CFL condition for both pure diffusion and pure advection by assigning $v = 0$ and $D = 0$ respectively.

Relation Between Flux Limiter and Mesh Parameters: From (13),

$$a = \frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x} - \frac{v\Delta t}{2\Delta x}\psi(r_{m-1}), \qquad c = \frac{D\Delta t}{\Delta x^2} - \frac{v\Delta t}{2\Delta x}\psi(r_m),$$
$$b = 1 - \frac{2D\Delta t}{\Delta x^2} - \frac{v\Delta t}{\Delta x} + \frac{v\Delta t}{2\Delta x}[\psi(r_{m-1}) + \psi(r_m)].$$

We shall represent $\psi(r_m)$ and $\psi(r_{m-1})$ in terms of general function $\psi(r)$. Substituting a, b and c in (15) and using $a + b + c = 1$, we have

$$4\left(1 - \frac{2D\Delta t}{\Delta x^2} - \frac{v\Delta t}{\Delta x} + \frac{v\Delta t}{\Delta x}(\psi(r)\right)\left(\frac{2D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x} - \frac{v\Delta t}{\Delta x}\psi(r)\right) \geq 0.$$

It is noted that $b \geq 0$ to preserve the positivity of the solution. Therefore,

$$1 - \frac{2D\Delta t}{\Delta x^2} - \frac{v\Delta t}{\Delta x} + \frac{v\Delta t}{\Delta x}(\psi(r) \geq 0$$

and

$$\frac{2D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x} - \frac{v\Delta t}{\Delta x}\psi(r) \geq 0$$

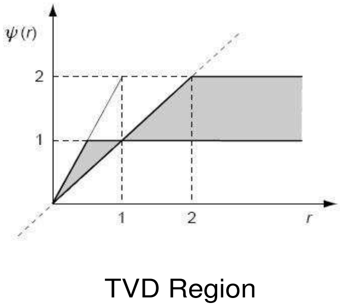


Figure 1: TVD region

which implies

$$1+\frac{2D}{v\Delta x}-\frac{\Delta x}{v\Delta t} \quad \le \psi(r) \le \quad 1+\frac{2D}{v\Delta x}. \tag{19}$$

The above condition indicates the stability of TVD schemes which gives the relationship between flux limiters and mesh parameters.

The TVD region of any limiter $\psi(r)$ is given by [20]

$$0 \quad \le \psi(r) \le \quad 2. \tag{20}$$

A TVD scheme will be stable if it satisfies both of the conditions (19) and (20). Combining these two conditions we have that, any lower bound and upper bound for the limiter should be less than or equal to 0 and greater than or equal to 2 respectively. Therefore, we have

$$1+\frac{2D}{v\Delta x}-\frac{\Delta x}{v\Delta t} \le 0 \quad \le \psi(r) \le \quad 2 \le 1+\frac{2D}{v\Delta x} \tag{21}$$

$$1+\frac{2D}{v\Delta x}-\frac{\Delta x}{v\Delta t} \le 0 \qquad\qquad 2 \le 1+\frac{2D}{v\Delta x}.$$

which eventually leads to,

$$\Delta x \le \frac{2D}{v} \qquad\qquad \Delta t \le \frac{\Delta x^2}{2D+v\Delta x}. \tag{22}$$

The above condition on mesh parameters will give the stable TVD schemes. The shaded portion in the Figure.1 is the TVD region. Any limiter falls in the region guarantees the variation diminishing schemes. The limiter $\psi(r)$ must be bounded by 0 and 2 when $r \to \infty$. If its not bounded by 0 and 2, we have to restrict the limiter in order to satisfy TVD region.

4. Truncation Error and Consistency

In this section, local truncation error and consistency of various schemes are discussed in detail.

Theorem 3. *Let $U_m^{n+1} = aU_{m-1}^n + bU_m^n + cU_{m+1}^n$ the general explicit finite difference scheme for the linear partial differential equation (1). The local truncation error of the scheme is given by*

$$\begin{aligned} T_{m,n} &= \frac{1}{\Delta t}\left[\Delta t\frac{\partial u}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2} - (a+b+c-1)u + (a-c)\Delta x\frac{\partial u}{\partial x}\right. \\ &- \left.(a+c)\frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\right]_{(x_m,t_n)} + \ldots \end{aligned}$$

The finite difference scheme is consistent with given partial differential equation (1) if $a+b+c=1$, $a-c=\frac{v\Delta t}{\Delta x}$ and $a+c=\frac{2D\Delta t}{\Delta x^{\mathbf{2}}}$.

Proof. The truncation error $T_{m,n}$ for the explicit scheme at interior nodal point (x_m, t_n) is defined by [18]

$$T_{m,n} = \frac{1}{\Delta t}\left[u(x_m, t_{n+1}) - U_m^{n+1}\right]$$

where $u(x_m, t_{n+1})$ and U_m^{n+1} are the values of exact and numerical solution at (x_m, t_{n+1}) respectively. Let $U_m^{n+1} = aU_{m-1}^n + bU_m^n + cU_{m+1}^n$, we have that

$$\Delta t T_{m,n} = u(x_m, t_{n+1}) - aU_{m-1}^n - bU_m^n - cU_{m+1}^n.$$

Following the usual procedure to obtain the truncation error, we replace numerical solution by exact solution

$$\begin{aligned} \Delta t T_{m,n} &= u(x_m, t_{n+1}) - au(x_{m-1}, t_n) - bu(x_m, t_n) - cu(x_{m+1}, t_n) \\ &= u(x_m, t_n + \Delta t) - au(x_m - \Delta x, t_n) - bu(x_m, t_n) \\ &- cu(x_m + \Delta x, t_n). \end{aligned}$$

Expanding using Taylor series , we have that

$$\begin{aligned} \Delta t \quad T_{m,n} = &\left\{\left[u + \Delta t\frac{\partial u}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2} + \ldots\right] - a\left[u - \Delta x\frac{\partial u}{\partial x}\right.\right. \\ + &\left.\left.\frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2} + \ldots\right] - bu - c\left[u + \Delta x\frac{\partial u}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2} + \ldots\right]\right\}_{(x_m,t_n)} \end{aligned}$$

$$\begin{aligned}
&= \left\{\Delta t\frac{\partial u}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2} - (a+b+c-1)u + (a-c)\Delta x\frac{\partial u}{\partial x}\right. \\
&- \left.(a+c)\frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\right\}_{(x_m,t_n)} + ... \\
&= \left\{\Delta t\frac{\partial u}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2} + (a-c)\Delta x\frac{\partial u}{\partial x} - (a+c)\frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\right. \\
&+ \left.(a-c)\frac{\Delta x^3}{6}\frac{\partial^3 u}{\partial x^3} + ...\right\}_{(x_m,t_n)} \text{ using } a+b+c=1. \qquad (23)
\end{aligned}$$

This implies that the local truncation error may be consistent with the given partial differential equation (1) $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - v\frac{\partial u}{\partial x}$ depending on $a+c$ and $a-c$. Let $a-c = \frac{v\Delta t}{\Delta x}$ and $a+c = \frac{2D\Delta t}{\Delta x^2}$. Then the scheme is consistent with given partial differential equation (1). □

Remark 4.1. We have that $a+b+c=1$ for central difference, upwind scheme and TVD schemes.

We shall discuss below the local truncation error and consistency for central difference, upwind and TVD schemes.

Truncation Error for Central Difference Scheme: Using $a-c = \frac{v\Delta t}{\Delta x}$ and $a+c = \frac{2D\Delta t}{\Delta x^2}$ from (10) in (23), we have

$$\begin{aligned}
\Delta t T_{m,n} &= \left[\Delta t\frac{\partial u}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2} + v\Delta t\frac{\partial u}{\partial x} - D\Delta t\frac{\partial^2 u}{\partial x^2}\right. \\
&+ \left.\frac{v\Delta t\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + ...\right]_{(x_m,t_n)}
\end{aligned}$$

$$\begin{aligned}
T_{m,n} &= \left\{\left[\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2}\right] + \left[\frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + \frac{v\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3}\right.\right. \\
&- \left.\left.\frac{D\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4} + ...\right]\right\}_{(x_m,t_n)} \qquad (24)
\end{aligned}$$

The first term of right hand side is the given partial differential equation evaluated at the interior point (x_m, t_n). Therefore, we have that

$$T_{m,n} = \left[\frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} + \frac{v\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} - \frac{D\Delta t\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4}\right] + ...$$

Hence, the order of truncation error is $O(\Delta t + \Delta x^2)$. If $\Delta t = \Delta x^2$, then the truncation error will be of $O(\Delta x^2)$. We therefore have that $\|u - U_h\|_\infty = O(h^2)$ where $h = \Delta x$ and U_h is numerical solution for the spatial discretization length h. For different values of h_2 and h_2, we have that

$$\frac{\|u - U_{h_1}\|_\infty}{\|u - U_{h_2}\|_\infty} \approx \left(\frac{h_1}{h_2}\right)^2$$

$$ie, \quad \frac{log\left(\frac{\|u-U_{h_1}\|_\infty}{\|u-U_{h_2}\|_\infty}\right)}{log\left(\frac{h_1}{h_2}\right)} \approx 2. \tag{25}$$

Therefore, the order of convergence of central difference scheme is two. Letting $\Delta t \to 0$ and $\Delta x \to 0$, the truncation error (24) $T_{m,n} \to 0$ and consistent with the partial differential equation (1).

Truncation Error for Upwind Scheme: Substituting $a - c = \frac{v\Delta t}{\Delta x}$ and $a + c = \frac{2D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x}$ from (12)in (23), we get truncation error for upwind scheme

$$\begin{aligned}\Delta t T_{m,n} &= \left[\Delta t\frac{\partial u}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2} + v\Delta t\frac{\partial u}{\partial x} - D\Delta t\frac{\partial^2 u}{\partial x^2}\right. \\ &- \left.\frac{v\Delta t\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + ...\right]_{(x_m,t_n)}\end{aligned}$$

$$\begin{aligned}T_{m,n} &= \left\{\left[\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2}\right] + \left[\frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} - \frac{v\Delta x}{2}\frac{\partial^2 u}{\partial x^2}\right.\right. \\ &- \left.\left.\frac{D\Delta x^2}{12}\frac{\partial^4 u}{\partial x^4} + ...\right]\right\}_{(x_m,t_n)}\end{aligned} \tag{26}$$

$$T_{m,n} = \frac{\Delta t}{2}u_{tt} + \frac{v\Delta x}{2}u_{xx} + ...$$

Here, the truncation error is of order $O(\Delta t + \Delta x)$. If $\Delta t = \Delta x$, then the truncation error will be of order $O(\Delta x)$. In a similar manner to central difference scheme, we have

$$\frac{log\left(\frac{\|u-U_{h_1}\|_\infty}{\|u-U_{h_2}\|_\infty}\right)}{log\left(\frac{h_1}{h_2}\right)} \le 1. \tag{27}$$

It means that upwind scheme is of first order convergence. Also, the truncation error (26) $T_{m,n} \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$ and consistent with the partial differential equation (1).

Truncation Error for TVD Scheme: Substituting $a+c = \frac{2D\Delta t}{\Delta x^2} + \frac{v\Delta t}{\Delta x} - \frac{v\Delta t}{\Delta x}\psi(r)$ and $a-c = \frac{v\Delta t}{\Delta x}$ from (13) in (23), we have

$$\begin{aligned} T_{m,n} &= \left\{ \left[\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} \right] + \left[[1-\psi(r)]\, \frac{v\Delta x}{2}\frac{\partial^2 u}{\partial x^2} + \frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2} \right.\right. \\ &+ \left.\left. \frac{v\Delta x^2}{6}\frac{\partial^3 u}{\partial x^3} + ... \right] \right\}_{(x_m,t_n)} \end{aligned} \tag{28}$$

Here, the order of truncation error is $O(\Delta t + \Delta x)$. The truncation error (28) $T_{m,n} \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$ and consistent with the partial differential equation (1). If $|1-\psi(r)| \le 1$ (ie, $0 \le \psi(r) \le 2$), then the numerical diffusion gets reduced. In this case, the truncation error approaches second order $O(\Delta t + \Delta x^2)$.

5. Results and Discussion

The numerical simulations are carried out for various limiters like central difference, upwind, linear upwind, UMIST, van Leer, van Albada, Minmod, Superbee, Sweby and Osher and then the results are compared with analytical solution (6). The error associated in the numerical approximation with respect to supremum norm is calculated for various schemes mentioned above.

The numerical concentration profile of chemical species simulated with initial concentration $u_0 = 100$, diffusion coefficient $D = 0.4$ and transport velocity $v = 0.1\ m\ h^{-1}$ obtained by various schemes for 225 hours. The constant β in Sweby and Osher limiter is assigned with the value $\beta = 1.5$. Further their Error of Convergence(EOC) are computed and shown in Table.3. The EOC is computed using the following formula

$$EOC = \frac{log\left(\frac{\|u-U_{h_i}\|_\infty}{\|u-U_{h_{i+1}}\|_\infty}\right)}{log\left(\frac{h_i}{h_{i+1}}\right)} \text{ for } i = 1, 2, 3.$$

The Lax theorem states that a linear numerical scheme is convergent if and only if it is stable and consistent. The central difference, upwind schemes and TVD schemes are stable with the stability condition discussed in Section 3.

Name	Limiter $\psi(r)$	Name	Limiter $\psi(r)$
Upwind	0	Min-Mod	$Max[0, Min(r, 1)]$
Central	1	Superbee	$Max[0, Min(2r, 1), Min(r, 2)]$
van Leer	$(r + \|r\|)/(1 + r)$	Sweby	$Max[0, Min(\beta r, 1), Min(r, \beta)]$
van Albada	$(r + r^2)/(1 + r^2)$	Osher	$Max[0, Min(r, \beta)]$ $1 \leq \beta \leq 2$
Linear UD	$Min(r, 2)$	Downwind	$Min(2r, 1)$
UMIST		$Max[0, Min(2r, (3 + r)/4, (1 + 3r)/4, 2)]$	

Table 1: Various flux limiters

It is proven that in Section 4, all the numerical schemes derived in Section 2 are consistent with the given partial differential equation (1). Therefore, the central difference, upwind and TVD schemes are convergent and their numerical solutions converge to exact solution. The theoretical results from Section 4 shows that the central difference scheme is of second order convergence where as the upwind scheme of first order convergence. Further, The order of convergence of TVD scheme lies between one to two. All the limiters of TVD schemes that are considered in the numerical experiment fall into the TVD region, hence a second order convergence is expected. The theoretical order of convergence of central difference, upwind and TVD schemes are validated by numerical order of convergence in Table.2. Further, it is evident from Table.2 that the order of TVD schemes approaches to two.

The conclusion is that the central difference scheme and TVD schemes are more accurate but it works for Peclet number less than two. The upwind scheme has first order convergence. Therefore, the numerical solution obtained by upwind scheme is not so closer to exact solution than that of obtained by central difference scheme and TVD schemes. But the great advantage of upwind scheme is that the stability condition is derived precisely from (18) and it can work for large Peclet numbers.

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Central Difference			Upwind		
h and $\triangle t = h^2$	$\|u - U_h\|_\infty$	EOC	h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC
1.0 and 1.0	0.298519	-	1.0 and 1.0	1.687546	-
1.5 and 2.25	0.621133	1.807089	1.5 and 1.5	2.476422	0.945915
2.5 and 6.25	1.575565	1.82219	2.5 and 2.5	3.935069	0.906597
3.0 and 9.0	2.22028	1.881404	3.0 and 3.0	4.634617	0.897456
van Albada			van Leer		
h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC	h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC
1.0 and 1.0	0.388266	-	1.0 and 1.0	0.383583	-
1.5 and 1.5	0.769415	1.686803	1.5 and 1.5	0.761637	1.691672
2.5 and 2.5	1.783781	1.646079	2.5 and 2.5	1.764573	1.6447746
3.0 and 3.0	2.345416	1.501344	3.0 and 3.0	2.322536	1.506925
Linear upwind			Minmod		
h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC	h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC
1.0 and 1.0	0.48505	-	1.0 and 1.0	0.423896	-
1.5 and 1.5	0.975618	1.7234997	1.5 and 1.5	0.829475	1.655641
2.5 and 2.5	2.272978	1.6557	2.5 and 2.5	1.861444	1.582368
3.0 and 3.0	3.020731	1.599924	3.0 and 3.0	2.413661	1.424911
Superbee			Sweby		
h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC	h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC
1.0 and 1.0	0.332284	-	1.0 and 1.0	0.333472	-
1.5 and 1.5	0.656498	1.679377	1.5 and 1.5	0.656768	1.671591
2.5 and 2.5	1.533504	1.660821	2.5 and 2.5	1.609383	1.75456
3.0 and 3.0	2.077721	1.665827	3.0 and 3.0	2.174518	1.650688
UMIST			Osher		
h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC	h and $\triangle t = h$	$\|u - U_h\|_\infty$	EOC
1.0 and 1.0	0.340151	-	1.0 and 1.0	0.486886	-
1.5 and 1.5	0.671218	1.673755	1.5 and 1.5	0.967759	1.6942344
2.5 and 2.5	1.530736	1.6138757	2.5 and 2.5	2.225618	1.6303134
3.0 and 3.0	1.998611	1.46282	3.0 and 3.0	2.935932	1.51924

Table 2: Order of convergence

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