Weighted Average Approximation in Finite Volume Formulation for One-Dimensional Single Species Transport and the Stability Condition for Various Schemes

S. Prabhakaran and L. Jones Tarcius Doss

Abstract The governing equation for one-dimensional single species transport model in a saturated porous medium with appropriate initial and boundary conditions is discretized by using finite volume formulation. A weighted average approximation is then applied to the integral terms. Twelve different schemes of explicit, semi-implicit, and fully implicit in nature are derived. The stability and convergence of those numerical schemes are also discussed. The numerical experiments are carried out for the single species transport problem with degradation in liquid phase. These numerical results are compared with the analytical solution. It is shown that semi-implicit and fully implicit type schemes are not always unconditionally stable. A novel numerical technique is used to approximate the reaction term of partial differential equation. Taking average for reaction term at different time levels yields a better approximation for upwind scheme. Further, it is proved that the averaging technique gives unconditional stability for implicit nature numerical schemes.

Keywords Finite volume method · Weighted average · Contamination transport · Stability · Consistency · First-order reaction

1 Introduction

In the modernized society, the use of chemicals becomes inevitable in day-to-day life. The chemical producing factories are growing like any other industry. The dumping of chemical waste by these factories spoils the surrounding soil of the earth and groundwater quality. The aquifers beneath the earth surface get contaminated more and more by reactive substances like petroleum hydrocarbons and chlorinated

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solvents. The chemical particles in the waste react with other minerals and metals beneath the surface. These reactions in the aquifers may pose great danger to nature. Therefore, there is a need to study reactive transport in a porous medium. Further, the study about contamination discharge is very important to protect groundwater, oil, and metals.

Analytical solutions for species transport models have been developed since 1971. Cho [1] described the analytical solution for the transport of ammonium with sequential first-order kinetic reaction. This is considered to be a pioneer paper in species transport. At the end of twentieth century, Sun and Clement [2] and Sun et al. [3] have developed a transport model involving the retardation factor. Latter, Bauer et al. [4] and Clement et al. [5] found an analytical solution for multi species transport with first-order sequential reaction involving distinct retardation factors. The analytical solutions are derived with the main assumption that the data set is continuous. But in many real-life problems, the data varies drastically. Therefore, analytical solutions are not so beneficial and hence computationally simulated solutions with the past information are useful for many physical problems.

The computational aspect purely depends on numerical techniques. There are various numerical techniques like finite difference, finite element, and finite volume used to solve equations arising from physical phenomena. A few well-known numerical techniques are listed below in the arena of species transport models. Clement [6] has applied finite difference method for the transport model and then developed a software RT3D. Many available groundwater simulating software like, MODFLOW, PLASAM, AQUIFEM, and FEFLOW are developed from either finite difference or finite element discretization. There are drawbacks in implementing these methods for property transport problems. The finite difference method is not advisable for complex geometry and flux boundary conditions. The finite element method has the global mass conservation property but not locally. The mass conservation principle is pretty important in any transport problem. The finite volume technique takes care of physical and chemical phenomena of the problem under consideration with its local mass conservation principle. In this article, an attempt has been made to study finite volume formulation for transport equation.

2 Governing Equation

The partial differential equation with the appropriate initial and boundary conditions which describes the single species transport in x-direction in a saturated porous medium is given below (see, [4]).
PDE:

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

Type of boundary conditions:

$$c(0,t) = C_0 \qquad t > 0 \tag{2}$$

$$c(0,t) = f(t) \qquad t > 0 \tag{3}$$

$$\lim_{x\to\infty} c(x,t) = 0 \qquad t > 0 \tag{4}$$

Type of initial conditions:

$$c(x,0) = 0 \qquad 0 < x < \infty \tag{5}$$

$$c(x,0) = (x)\ with\ \lim_{x\to\infty} g(x) = 0 \tag{6}$$

Here, c is the concentration of species [ML^{-3}]; R, the retardation factor; v, the prescribed constant transport velocity in x direction [LT^{-1}]; k, the first-order contaminant destruction rate constant [T^{-1}]; and D, the dispersion coefficient [$L^{-1}T^{-1}$].

The problem is to find the concentration of a species $c(x, t)$ at any distance x measured from the origin in any time t satisfying above PDE, initial, and boundary conditions. The boundary condition (2) represents the source of constant dumping of chemical wastage, whereas (3) represents the varying dumping in time t. The condition (4) indicates the zero concentration of species at the farther end at infinity. Similarly, the initial condition (5) represents that there is no sign of species concentration (i.e., contamination) at the initial time. The alternate condition (6) indicates the initial presence of contamination.

The kinetics of reaction is assumed to be of first order. The radioactive decay is an example for a true first-order process. Also chemical and biological transforms can be approximately treated as first-order reaction. Equation (1) assumes that degradation occurs only in the liquid phase.

The above transport equation (1) is used for solving different types of environmental problems. Bauer et al. [4] utilized to model transport of decay chain in homogeneous porous media. Clement et al. [5] applied the generalized form to model multi-species transport coupled with first-order reaction network with distinct retardation factors. The similar kind of equations are employed to model the fate and transport of chlorinated solvent plumes by Clement et al. [7, 8]. Cho [1] used it to model the fate and transport of nitrate species in soil–water systems; Van Genuchten [9] applied it for modeling radionuclide migration. Elango et al. [10] used for groundwater flow and radionuclide decay-chain transport modeling around a proposed uranium tailing pond in India.

Result 2.1

Analytical solution to species transport equation (1) with conditions (2), (4) and (5) is given by (see, [5]):

$$c(x,t) = \frac{C_0}{2}\exp\left(\frac{vx}{2D}\right)\left[\exp\left(-\frac{mx}{2D}\right) erfc\left(\frac{Rx - mt}{\sqrt{4DRt}}\right) + \exp\left(\frac{mx}{2D}\right) erfc\left(\frac{Rx + mt}{\sqrt{4DRt}}\right)\right], \tag{7}$$

where $m = \sqrt{u^2 + 4kD}$.

3 Derivation of the Numerical Scheme

In this section, a finite volume formulation is presented for the transport equation (2.1) described in previous section. The computational domain is discretized by non overlapping control volumes. The control volume (CV) is given in Fig. 1.

Here, $\Delta V = A\Delta x$. Where A is cross-sectional area and Δx is the spatial discretization length. W, P and E are western, present and eastern nodal points. w and e are western and eastern faces of control volume. Though the control volume is in three-dimensional space, only one-dimensional (i.e., x-direction) transport problem is considered in this paper. Therefore, the other two dimensions are assumed to be negligible.
The vector form of (1) is given by

$$R\frac{\partial c}{\partial t} = \overline{\nabla} \cdot (\overline{\nabla} Dc) - \overline{v} \cdot \overline{\nabla}(c) - kc. \tag{8}$$

Integrating the above PDE over the control volume in the interval $(t, t + \Delta t)$ with time step Δt and then applying Gauss divergence theorem, we obtain

$$R\int_t^{t+\Delta t}\int_{CV}\frac{\partial c}{\partial t}dVdt = \int_t^{t+\Delta t}\int_{CV}\overline{\nabla}\cdot(\overline{\nabla}Dc)dVdt - \int_t^{t+\Delta t}\int_{CV}\overline{v}\cdot\overline{\nabla}(c)dVdt - \int_t^{t+\Delta t}\int_{CV}kcdVdt.$$

$$R\int_{CV}(c^{n+1}-c^n)dV = \int_t^{t+\Delta t}\int_S\overrightarrow{n}\cdot\overline{\nabla}(Dc)dSdt - \int_t^{t+\Delta t}\int_S\overrightarrow{n}\cdot(c\overline{v})dSdt - C_{avg}k\int_{CV}dV\int_t^{t+\Delta t}dt,$$

where $\overrightarrow{n}$ is the outward normal to the surface S (cross-sectional area A) and C_{avg} is the average concentration c inside CV. One-dimensional formulation of above integral is given by

$$R\int_{CV}(c^{n+1}-c^n)dV = \int_t^{t+\Delta t}\int_S\overrightarrow{n}\cdot\overline{i}\frac{\partial(Dc)}{\partial x}dSdt - \int_t^{t+\Delta t}\int_S\overrightarrow{n}\cdot\overline{i}(cv)dSdt - C_{avg}kA\Delta x\Delta t,$$

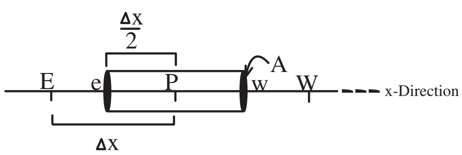

Fig. 1 Control volume (CV)

where C_P^n be the approximation of $c(x,t)$ at the nodal point (x_p, t_n). The parameters D and v are assumed to be constants. Using weighted average for the time integration to obtain

$$R(C_P^{n+1}-C_P^n)\Delta x = \left[(1-\theta)\left[\left(\frac{\partial c}{\partial x}\right)_e^n - \left(\frac{\partial c}{\partial x}\right)_w^n\right] + \theta\left[\left(\frac{\partial c}{\partial x}\right)_e^{n+1} - \left(\frac{\partial c}{\partial x}\right)_w^{n+1}\right]\right] D\Delta t$$
$$-\left[(1-\theta)[c_e^n - c_w^n] - \theta[c_e^{n+1} - c_w^{n+1}]\right] v\Delta t - C_{avg} k \Delta x \Delta t.$$

Using the following central difference approximation for the derivative term

$$\left(\frac{\partial c}{\partial x}\right)_e^n \approx \frac{C_E^n - C_P^n}{\Delta x} \qquad \left(\frac{\partial c}{\partial x}\right)_w^n \approx \frac{C_P^n - C_W^n}{\Delta x},$$

we obtain

$$R(C_P^{n+1}-C_P^n)\Delta x = (1-\theta)\frac{D\Delta t}{\Delta x}\left[C_W^n - 2C_P^n + C_E^n\right] + \theta\frac{D\Delta t}{\Delta x}\left[C_W^{n+1} - 2C_P^n + C_E^{n+1}\right]$$
$$-(1-\theta)v\Delta t\left[c_e^n - c_w^n\right] - \theta v\Delta t\left[c_e^{n+1} - c_w^{n+1}\right] - C_{avg} k\Delta x\Delta t. \quad (9)$$

4 Various Numerical Schemes

The following 12 different numerical schemes are derived for different values of θ and different approximations to C_{avg} and C_{Face}.

θ-values	$C_{Average}$	C_{Face}	Scheme
$\theta = 0$	$C_{avg} = C_P^n$	$C_e^n = \frac{C_E^n + C_P^n}{2}, C_w^n = \frac{C_P^n + C_W^n}{2}$	Scheme 1
		$C_e^n = C_P^n, C_w^n = C_W^n$	Scheme 3
	$C_{avg} = \frac{C_P^n + C_P^{n+1}}{2}$	$C_e^n = \frac{C_E^n + C_P^n}{2}, C_w^n = \frac{C_P^n + C_W^n}{2}$	Scheme 2
		$C_e^n = C_P^n, C_w^n = C_W^n$	Scheme 4
$\theta = \frac{1}{2}$	$C_{avg} = C_P^n$	$C_e^n = \frac{C_E^n + C_P^n}{2}, C_w^n = \frac{C_P^n + C_W^n}{2}$	Scheme 5
		$C_e^n = C_P^n, C_w^n = C_W^n$	Scheme 7
	$C_{avg} = \frac{C_P^n + C_P^{n+1}}{2}$	$C_e^n = \frac{C_E^n + C_P^n}{2}, C_w^n = \frac{C_P^n + C_W^n}{2}$	Scheme 6
		$C_e^n = C_P^n, C_w^n = C_W^n$	Scheme 8
$\theta = 1$	$C_{avg} = C_P^n$	$C_e^n = \frac{C_E^n + C_P^n}{2}, C_w^n = \frac{C_P^n + C_W^n}{2}$	Scheme 9
		$C_e^n = C_P^n, C_w^n = C_W^n$	Scheme 11
	$C_{avg} = \frac{C_P^n + C_P^{n+1}}{2}$	$C_e^n = \frac{C_E^n + C_P^n}{2}, C_w^n = \frac{C_P^n + C_W^n}{2}$	Scheme 10
		$C_e^n = C_P^n, C_w^n = C_W^n$	Scheme 12

The approximations $C_e^n = C_P^n, C_w^n = C_W^n$ and $C_e^n = C_P^n, C_w^n = C_W^n$ are called central difference and upwind, respectively. The average of concentration $C_{avg} = \frac{C_P^n + C_P^{n+1}}{2}$ at n and $n+1$ time level is justified because the control volume is fixed. Following explicit schemes are obtained by substituting $\theta = 0$.

Explicit type schemes ($\theta = 0$)
Scheme 1

$$C_P^{n+1} = \left[\frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{2R\Delta x}\right]C_W^n + \left[1 - \frac{2D\Delta t}{R\Delta x^2} - \frac{k\Delta t}{R}\right]C_P^n + \left[\frac{D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x}\right]C_E^n. \quad (10)$$

Scheme 2

$$\left[1 + \frac{k\Delta t}{2R}\right]C_P^{n+1} = \left[\frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{2R\Delta x}\right]C_W^n + \left[1 - \frac{2D\Delta t}{R\Delta x^2} - \frac{k\Delta t}{2R}\right]C_P^n + \left[\frac{D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x}\right]C_E^n. \quad (11)$$

Scheme 3

$$C_P^{n+1} = \left[\frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{R\Delta x}\right]C_W^n + \left[1 - \frac{2D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{R\Delta x} - \frac{k\Delta t}{R}\right]C_P^n + \left[\frac{D\Delta t}{R\Delta x^2}\right]C_E^n. \quad (12)$$

Scheme 4

$$\left[1 + \frac{k\Delta t}{2R}\right]C_P^{n+1} = \left[\frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{R\Delta x}\right]C_W^n + \left[1 - \frac{2D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{R\Delta x} - \frac{k\Delta t}{2R}\right]C_P^n + \left[\frac{D\Delta t}{R\Delta x^2}\right]C_E^n. \quad (13)$$

For $\theta = \frac{1}{2}$, we have the following schemes.

Semi-implicit type schemes ($\theta = \frac{1}{2}$)

Scheme 5

$$-\left[\frac{D\Delta t}{2R\Delta x^2} + \frac{v\Delta t}{4R\Delta x}\right]C_W^{n+1} + \left[1 + \frac{D\Delta t}{R\Delta x^2}\right]C_P^{n+1} - \left[\frac{D\Delta t}{2R\Delta x^2} - \frac{v\Delta t}{4R\Delta x}\right]C_E^{n+1}$$
$$= \left[\frac{D\Delta t}{2R\Delta x^2} + \frac{v\Delta t}{4R\Delta x}\right]C_W^n + \left[1 - \frac{D\Delta t}{R\Delta x^2} - \frac{k\Delta t}{R}\right]C_P^n + \left[\frac{D\Delta t}{2R\Delta x^2} - \frac{v\Delta t}{4R\Delta x}\right]C_E^n. \quad (14)$$

Scheme 6

$$-\left[\frac{D\Delta t}{2R\Delta x^2} + \frac{v\Delta t}{4R\Delta x}\right]C_W^{n+1} + \left[1 + \frac{D\Delta t}{R\Delta x^2} + \frac{k\Delta t}{2R}\right]C_P^{n+1} - \left[\frac{D\Delta t}{2R\Delta x^2} - \frac{v\Delta t}{4R\Delta x}\right]C_E^{n+1}$$
$$= \left[\frac{D\Delta t}{2R\Delta x^2} + \frac{v\Delta t}{4R\Delta x}\right]C_W^n + \left[1 - \frac{D\Delta t}{R\Delta x^2} - \frac{k\Delta t}{2R}\right]C_P^n + \left[\frac{D\Delta t}{2R\Delta x^2} - \frac{v\Delta t}{4R\Delta x}\right]C_E^n. \quad (15)$$

Scheme 7

$$-\left[\frac{D\Delta t}{2R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}\right]C_W^{n+1}+\left[1+\frac{D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}\right]C_P^{n+1}-\left[\frac{D\Delta t}{2R\Delta x^2}\right]C_E^{n+1}$$
$$=\left[\frac{D\Delta t}{2R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}\right]C_W^{n}+\left[1-\frac{D\Delta t}{R\Delta x^2}-\frac{v\Delta t}{2R\Delta x}-\frac{k\Delta t}{R}\right]C_P^{n}+\left[\frac{D\Delta t}{2R\Delta x^2}\right]C_E^{n}. \quad (16)$$

Scheme 8

$$-\left[\frac{D\Delta t}{2R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}\right]C_W^{n+1}+\left[1+\frac{D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}+\frac{k\Delta t}{2R}\right]C_P^{n+1}-\left[\frac{D\Delta t}{2R\Delta x^2}\right]C_E^{n+1}$$
$$=\left[\frac{D\Delta t}{2R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}\right]C_W^{n}+\left[1-\frac{D\Delta t}{R\Delta x^2}-\frac{v\Delta t}{2R\Delta x}-\frac{k\Delta t}{2R}\right]C_P^{n}+\left[\frac{D\Delta t}{2R\Delta x^2}\right]C_E^{n}. \quad (17)$$

Implicit type schemes ($\theta = 1$)

Scheme 9

$$-\left[\frac{D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}\right]C_W^{n+1}+\left[1+\frac{2D\Delta t}{R\Delta x^2}\right]C_P^{n+1}-\left[\frac{D\Delta t}{R\Delta x^2}-\frac{v\Delta t}{2R\Delta x}\right]C_E^{n+1}=\left[1-\frac{k\Delta t}{R}\right]C_P^{n}. \quad (18)$$

Scheme 10

$$-\left[\frac{D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{2R\Delta x}\right]C_W^{n+1}+\left[1+\frac{2D\Delta t}{R\Delta x^2}+\frac{k\Delta t}{2R}\right]C_P^{n+1}-\left[\frac{D\Delta t}{R\Delta x^2}-\frac{v\Delta t}{2R\Delta x}\right]C_E^{n+1}$$
$$=\left[1-\frac{k\Delta t}{2R}\right]C_P^{n}. \quad (19)$$

Scheme 11

$$-\left[\frac{D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{R\Delta x}\right]C_W^{n}+\left[1+\frac{2D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{R\Delta x}\right]C_P^{n}-\left[\frac{D\Delta t}{R\Delta x^2}\right]C_E^{n}=\left[1-\frac{k\Delta t}{R}\right]C_P^{n}. \quad (20)$$

Scheme 12

$$-\left[\frac{D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{R\Delta x}\right]C_W^{n}+\left[1+\frac{2D\Delta t}{R\Delta x^2}+\frac{v\Delta t}{R\Delta x}+\frac{k\Delta t}{2R}\right]C_P^{n}-\left[\frac{D\Delta t}{R\Delta x^2}\right]C_E^{n}=\left[1-\frac{k\Delta t}{2R}\right]C_P^{n}. \quad (21)$$

5 Stability Analysis

In this section, we shall discuss the stability of general form of the explicit, semi-implicit, and implicit finite difference schemes. The general form of explicit, semi-implicit, and implicit schemes are given below:

$$C_m^{n+1} = pC_{m-1}^n + qC_m^n + rC_{m+1}^n \tag{22}$$

$$-pC_{m-1}^{n+1} + qC_m^{n+1} - rC_{m+1}^{n+1} = pC_{m-1}^n + sC_m^n + rC_{m+1}^n \tag{23}$$

$$-pC_{m-1}^{n+1} + qC_m^{n+1} - rC_{m+1}^{n+1} = sC_m^n \tag{24}$$

Definition 5.1 A scheme $U_m^{n+1} = G(U_{m-k}^n, ..., U_m^n, ...U_{m+p}^n)$ is called monotone scheme if G is non-decreasing function of each of its argument.
i.e., $\frac{\partial G}{\partial U_i}(U_{-k}, ..., U_0, ...U_p) \geq 0, i = -k, ..., p.$

Theorem 5.1 *Let $C_m^{n+1} = pC_{m-1}^n + qC_m^n + rC_{m+1}^n$ be the general form of explicit finite difference scheme for the linear time-dependent partial differential equation (1). If $p \geq 0,\ q \geq 0$ and $r \geq 0$ and satisfy $(p+q+r)^2 \leq 1 + 4q(p+r)$, then the scheme is stable and monotone.*

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

$$\xi = pe^{-i\theta} + q + re^{i\theta} = q + (p+r)(\cos\theta) + i(r-p)\sin\theta.$$

The numerical scheme (22) is stable only when $|\xi| \leq 1$ which is equivalently $|\xi|^2 \leq 1$ (Smith, [11]). Therefore,

$$\begin{aligned} q^2 + (p+r)^2\cos^2\theta + 2q(p+r)\cos\theta + (r-p)^2\sin^2\theta &\leq 1 \\ \Leftrightarrow p^2 + q^2 + r^2 + 2pr(\cos^2\theta - \sin^2\theta) + 2q(p+r)\cos\theta &\leq 1 \\ \Leftrightarrow (p+q+r)^2 - 2q(p+r)(1-\cos\theta) - 2pr(1-\cos 2\theta) &\leq 1 \end{aligned}$$

$$\begin{aligned} &\Leftrightarrow (p+q+r)^2 \leq 1 + 4b(p+r)\sin^2\frac{\theta}{2} + 4pr\sin^2\theta \\ &\Leftrightarrow (p+q+r)^2 \leq 1 + 4q(p+r)\sin^2\frac{\theta}{2} + 16pr\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2} \\ \Leftrightarrow (p+q+r)^2 + 16pr\sin^4\frac{\theta}{2} &\leq 1 + 4q(p+r)\sin^2\frac{\theta}{2} + 16pr\sin^2\frac{\theta}{2}. \end{aligned}$$

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

$$(p+q+r)^2 \leq 1+4q(p+r). \tag{25}$$

Let us assume that p, q and r are greater than or equal to zero $(p, q, r \geq 0)$. Let $G(C^n_{m-1}, C^n_m, C^n_{m+1}) = pC^n_{m-1} + qC^n_m + rC^n_{m+1}$ be the function. From (22), $C^{n+1}_m = G(C^n_{m-1}, C^n_m, C^n_{m+1})$. By Definition (5.1) $\frac{\partial G}{\partial C_i}(C_{-1}, C_0, C_1) \geq 0, i = -1, 0, 1$, which implies that the scheme is monotone. Therefore, the monotone scheme which satisfies (25) is stable.

Theorem 5.2 *Let* $-pC^{n+1}_{m-1} + qC^{n+1}_m - rC^{n+1}_{m+1} = pC^n_{m-1} + sC^n_m + rC^n_{m+1}$ *be the general form of semi-implicit finite difference scheme for the time-dependent linear partial differential equation (1). If* $q+s > 0$, $q \geq s$ *and satisfy* $2(p+r) \leq q-s$, *then the scheme is stable.*

Proof Let $-pC^{n+1}_{m-1} + qC^{n+1}_m - rC^{n+1}_{m+1} = pC^n_{m-1} + sC^n_m + rC^n_{m+1}$ be any general semi-implicit scheme. Let $C^n_m = B\xi^n e^{im\theta}$. The von Neumann stability condition $|\xi| \leq 1$ implies

$$\begin{aligned}
\mid s+(p+r)(\cos\theta)+i(r-p)\sin\theta \mid &\leq \mid q-(p+r)(\cos\theta)+i(p-r)\sin\theta \mid \\
s^2+2s(p+r)\cos\theta &\leq q^2-2q(p+r)\cos\theta \\
2(q+s)(p+r)\cos\theta &\leq q^2-s^2 \\
2(q+s)(p+r)\cos\theta &\leq (q+s)(q-s)
\end{aligned}$$

Let us assume that $p+r \geq 0$, $(q+s) \geq 0$ and $q \geq s$. Maximizing with respect to θ, we obtain

$$2(p+r) \leq q-s \tag{26}$$

Therefore, any semi-implicit numerical scheme is of the form (23) which satisfies the condition (26) is stable.

Theorem 5.3 *Let* $-pC^{n+1}_{m-1} + qC^{n+1}_m - rC^{n+1}_{m+1} = sC^n_m$ *be the general form of implicit finite difference scheme for the linear time-dependent partial differential equation (1). If* $s^2 \leq (p+q+r)^2 - 4q(p+r)$, *then the scheme is stable.*

Proof Let $-pC^{n+1}_{m-1} + qC^{n+1}_m - rC^{n+1}_{m+1} = sC^n_m$ be the general form of implicit finite difference numerical scheme. Let $C^n_m = B\xi^n e^{im\theta}$. The von Neumann stability analysis for the above difference scheme implies

$$\xi(-pe^{-i\theta} + q - re^{i\theta}) = s.$$

$$\begin{aligned}
& s^2 \leq (p+r)^2\cos^2\theta - 2q(p+r)\cos\theta + q^2 + (p-r)^2\sin^2\theta \\
\Leftrightarrow\ & s^2 \leq p^2+q^2+r^2+2pr(\cos^2\theta - \sin^2\theta) - 2q(p+r)\cos\theta \\
\Leftrightarrow\ & s^2 \leq p^2+q^2+r^2+2pr(2\cos^2\theta - 1) - 2q(p+r)\cos\theta \\
\Leftrightarrow\ & s^2 \leq (p+q+r)^2+4pr(\cos^2\theta - 1) - 2q(p+r)(1+\cos\theta)
\end{aligned}$$

$$\Leftrightarrow s^2 + 4pr + 2q(p+r)(1+\cos\theta) \leq (p+q+r)^2 + 4pr\cos^2\theta$$

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

$$s^2 \leq (p+q+r)^2 - 4q(p+r). \tag{27}$$

Therefore, any implicit numerical scheme is of the form (24) which satisfies the condition (27) is stable.

Stability for explicit schemes
Comparing *Scheme 1* (10) with general form of explicit schemes (22), we have

$$p = \frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{2R\Delta x} \qquad q = 1 - \frac{2D\Delta t}{R\Delta x^2} - \frac{k\Delta t}{R} \qquad r = \frac{D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x}$$

$$p+q+r = 1 - \frac{k\Delta t}{R} \qquad 4q(p+r) = \frac{8D\Delta t}{R\Delta x^2} - \frac{16D^2\Delta t^2}{R^2\Delta x^4} - \frac{8Dk\Delta t^2}{R^2\Delta x^2}$$

Stability condition (25) implies

$$\Delta t \leq \frac{R(8D + 2k\Delta x^2)\Delta x^2}{16D^2 + k^2\Delta x^4 + 8Dk\Delta x^2} \tag{28}$$

The above condition is independent of velocity term v. Therefore, the stability behavior of central difference scheme can not judged. It should be noted that the condition (28) coincides with CFL condition for pure diffusion (i.e., $v = 0$ and $k = 0$) process. It is assumed that the coefficients of explicit schemes are greater than or equal to zero. Therefore, the coefficient $r \geq 0$ which is eventually

$$\frac{v\Delta x}{D} \leq 2 \tag{29}$$

The left-side quantity in above is nothing but the Peclet number. Therefore, the central difference scheme is stable for Peclet number less than or equal 2. For a pure reaction process (i.e., $D = 0$ and $v = 0$), the numerical scheme (10) becomes Euler method for first-order differential equation

$$C^{n+1} = \left[1 - \frac{k\Delta t}{R}\right] C^n.$$

And the stability condition (28) coincides with absolutely stable condition for Euler method which is given by

$$\left|1 - \frac{k\Delta t}{R}\right| \leq 1$$

The above condition may lead to produce negative result in the concentration profile in the explicit scheme (10). The positivity of the solution is important. Therefore, it should satisfy

$$0 \le 1 - \frac{k\Delta t}{R} \le 1$$
$$\text{i.e.,} \frac{k\Delta t}{R} \le 1 \tag{30}$$

for (10). The conditions (28) and (30) combined together will produce stable and positive solution for (10). Similarly, the stability condition for (11) is given by

$$p = \frac{\frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{2R\Delta x}}{1 + \frac{k\Delta t}{2R}} \qquad q = \frac{1 - \frac{2D\Delta t}{R\Delta x^2} - \frac{k\Delta t}{2R}}{1 + \frac{k\Delta t}{2R}} \qquad r = \frac{\frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{2R\Delta x}}{1 + \frac{k\Delta t}{2R}}$$

$$\Delta t \le \frac{R(8D + 4k\Delta x^2)\Delta x^2}{16D^2 + 8Dk\Delta x^2}. \tag{31}$$

$$\frac{v\Delta x}{D} \le 2$$

and

$$0 \le 1 - \frac{k\Delta t}{2R} \le 1$$

i.e.,

$$\frac{k\Delta t}{R} \le 2.$$

The stability conditions for (12) and (13) can be derived in the similar manner. The conditions for *Scheme 3* is given by

$$\Delta t \le \frac{R(8D + 4v\Delta x + 2k\Delta x^2)\Delta x^2}{16D^2 + 16Dv\Delta x + 8Dk\Delta x^2 + 4vk\Delta x^3 + 4v^2\Delta x^2 + k^2\Delta x^4}. \tag{32}$$

The above condition satisfies the CFL condition for pure diffusion and advection process. Also it satisfies absolute stability condition for Euler method for pure reaction process. The condition for *Scheme 4* is given by

$$\Delta t \le \frac{R(8D + 4v\Delta x + 4k\Delta x^2)\Delta x^2}{16D^2 + 16Dv\Delta x + 8Dk\Delta x^2 + 4vk\Delta x^3 + 4v^2\Delta x^2}. \tag{33}$$

In general, the first-order reaction co-efficient (k) is very small. Therefore, the contribution of k in the stability of explicit schemes is negligible. One must ensure that

$\frac{k\Delta t}{R} \leq 1$ for *scheme 1* and *scheme 3* and $\frac{k\Delta t}{R} \leq 2$ for *scheme 2* and *scheme 4* before implementation.

Stability for semi-implicit schemes

The semi-implicit type schemes *scheme 5, 6, 7* and *8* satisfy the condition (26). However the assumptions in Theorem 5.2 are not satisfied by all schemes. Only the two schemes, namely, *scheme 6* and *scheme 8* satisfy all assumptions. Therefore, they are unconditionally stable. *Scheme 5* and *scheme 7* satisfy all assumptions except $q + s \geq 0$. The condition $q + s \geq 0$ implies that

$$\frac{k\Delta t}{R} \leq 2.$$

Therefore, *scheme 5* and *scheme 7* are conditionally stable.

Stability for implicit schemes

Comparing *Scheme 9* (18) with general form of implicit schemes (24), we have

$$p = \frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{2R\Delta x} \qquad q = 1 + \frac{2D\Delta t}{R\Delta x^2} \qquad r = \frac{D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x} \qquad s = 1 - \frac{k\Delta t}{R}.$$

Stability condition (27) implies that

$$\begin{aligned}
\left(1 - \frac{k\Delta t}{R}\right)^2 &\leq \left(1 + \frac{4D\Delta t}{R\Delta x^2}\right)^2 - 4\left(1 + \frac{2D\Delta t}{R\Delta x^2}\right)\left(\frac{2D\Delta t}{R\Delta x^2}\right) \\
\left(1 - \frac{k\Delta t}{R}\right)^2 &\leq 1 \\
-1 \leq 1 - \frac{k\Delta t}{R} &\leq 1.
\end{aligned}$$

Therefore, *Scheme 9* is stable if $\frac{k\Delta t}{R} \leq 2$. Similarly, *Scheme 11* is also stable if $\frac{k\Delta t}{R} \leq 2$. The stability condition for *Scheme 10* is given by

$$p = \frac{D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{2R\Delta x} \qquad q = 1 + \frac{2D\Delta t}{R\Delta x^2} + \frac{k\Delta t}{2R} \qquad r = \frac{D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x} \qquad s = 1 - \frac{k\Delta t}{2R}.$$

Stability condition (27) implies that

$$\begin{aligned}
\left(1 - \frac{k\Delta t}{2R}\right)^2 &\leq \left(1 + \frac{4D\Delta t}{R\Delta x^2} + \frac{k\Delta t}{2R}\right)^2 - 4\left(1 + \frac{2D\Delta t}{R\Delta x^2} + \frac{k\Delta t}{2R}\right)\left(\frac{2D\Delta t}{R\Delta x^2}\right) \\
\left(1 - \frac{k\Delta t}{R}\right)^2 &\leq \left(1 + \frac{k\Delta t}{R}\right)^2 \\
0 &\leq \frac{4k\Delta t}{R}.
\end{aligned}$$

Therefore, *Scheme 10* is unconditionally stable. Similarly, *Scheme 12* is also unconditionally stable.

6 Truncation Error and Consistency

The truncation error $T_{i,j}$ at interior nodal point (x_i, t_j) is defined by

$$T_{i,j} = pC_{i-1}^{j+1} + qC_i^{j+1} + rC_{i+1}^{j+1} - aC_{i-1}^{j} - bC_i^{j} - dC_{i+1}^{j}$$

where C_i^j is the solution at (x_i, t_j). Following the usual procedure to obtain the truncation error, we replace numerical solution by exact solution

$$\begin{aligned} T_{i,j} &= pc_{i-1}^{j+1} + qc_i^{j+1} + rc_{i+1}^{j+1} - aC_{i-1}^{j} - bC_i^{j} - dC_{i+1}^{j} \\ &= pc(x_i - \Delta x, t_j + \Delta t) + qc(x_i, t_j + \Delta t) + rc(x_i + \Delta x, t_j + \Delta t) \\ &\quad -ac(x_i - \Delta x, t_j) - bc(x_i, t_j) - dc(x_i + \Delta x, t_j). \end{aligned}$$

Expanding using Taylor series, we have that

$$\begin{aligned} T_{i,j} = &\left\{ (p+q+r-a-b-d)c + (p+q+r)\left[\Delta t \frac{\partial c}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 c}{\partial t^2} + \cdots \right] \right\}_{(x_i,t_j)} \\ &+ \left\{ (r-p-d+a)\left[\Delta x \frac{\partial c}{\partial x} + \frac{\Delta x^3}{6}\frac{\partial^3 c}{\partial x^3} \right] + (r+p-d-a)\frac{\Delta x^2}{2}\frac{\partial^2 c}{\partial x^2} \right\}_{(x_i,t_j)} \\ &+ \left\{ (r-p)\left[\Delta x \Delta t \frac{\partial^2 c}{\partial x \partial t} + \frac{\Delta x \Delta t^2}{2}\frac{\partial^3 c}{\partial x \partial t^2} \right] + (r+p)\frac{\Delta x^2 \Delta t}{2}\frac{\partial^3 c}{\partial x^2 \partial t} + \cdots \right\}_{(x_i,t_j)} \end{aligned} \tag{34}$$

Explicit type schemes

Scheme 1

From (10), $p = r = 0$, $q = 1$, $a + b + d = 1 - \frac{k\Delta t}{R}$, $a - d = \frac{v\Delta t}{R\Delta x}$ and $a + d = \frac{2D\Delta t}{R\Delta x^2}$. Using these in (34), We have that

$$T_{i,j} = \left[\frac{kc\Delta t}{R} + \Delta t\frac{\partial c}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 c}{\partial t^2} + \frac{v\Delta t}{R}\frac{\partial c}{\partial x} - \frac{D\Delta t}{R}\frac{\partial^2 c}{\partial x^2} + \frac{v\Delta t\Delta x^2}{6R}\frac{\partial^3 c}{\partial x^3}\right]_{(x_i,t_j)} + \cdots$$

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2}\right]_{(x_i,t_j)} + \left[\frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} + \frac{v\Delta x^2}{6R}\frac{\partial^3 c}{\partial x^3}\right]_{(x_i,t_j)} + \cdots \tag{35}$$

The first term of right hand side is the given partial differential equation (1) evaluated at the interior point (x_i, t_j). Therefore, we have that

$$\frac{1}{\Delta t}T_{i,j} = \frac{\Delta t}{2}c_{tt} + \frac{v\Delta x^2}{6R}c_{xxx} + \cdots$$

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 $O(\Delta x^2)$. There fore, $\|c - C_h\|_\infty = O(h^2)$, where $h = \Delta x$ is order and C_h is numerical solution for the mesh length h. For different mesh lengths h_2 and h_2, we have that

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

$$\text{i.e., } \frac{\log\left(\frac{\|c-C_{h_1}\|_\infty}{\|c-C_{h_2}\|_\infty}\right)}{\log\left(\frac{h_1}{h_2}\right)} \approx 2 \tag{36}$$

Therefore, the order of convergence of *Scheme 1* is two. Let $\Delta t \to 0$ and $\Delta x \to 0$, the truncation error (35) $T_{i,j} \to 0$, the scheme is consistent with the partial differential equation (1).

Scheme 2

From (11), $p = r = 0, q = 1 + \frac{k\Delta t}{2R}, a + b + d = 1 - \frac{k\Delta t}{2R}, a - d = \frac{v\Delta t}{R\Delta x}$ and $a + d = \frac{2D\Delta t}{R\Delta x^2}$ in Eq. (34), We have

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2}\right]_{(x_i,t_j)} + \left[\frac{k\Delta t}{2R}\frac{\partial c}{\partial t} + \frac{v\Delta x^2}{6R}\frac{\partial^3 c}{\partial x^3}\right]_{(x_i,t_j)} + \cdots \tag{37}$$

which implies that

$$\frac{1}{\Delta t}T_{i,j} = \frac{k\Delta t}{2R}c_t + \frac{v\Delta x^2}{6R}c_{xxx} + \cdots$$

The local truncation error is $O(\Delta t + \Delta x^2)$ and its order is two. Also the scheme is consistent with the partial differential equation (1).

Scheme 3

Substituting $p = r = 0$, $q = 1$, $a + b + d = 1 - \frac{k\Delta t}{R}$, $a - d = \frac{v\Delta t}{R\Delta x}$ and $a + d = \frac{2D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{R\Delta x}$ in (34), we get truncation error for *Scheme 3*

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2}\right]_{(x_i,t_j)} + \left[\frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} - \frac{v\Delta x}{2R}\frac{\partial^2 c}{\partial x^2}\right]_{(x_i,t_j)} + \cdots \quad . \tag{38}$$

$$\frac{1}{\Delta t}T_{i,j} = \frac{\Delta t}{2}c_{tt} - \frac{v\Delta x}{2R}c_{xx} + \cdots$$

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

$$\frac{log\left(\frac{\|c - C_{h_1}\|_\infty}{\|c - C_{h_2}\|_\infty}\right)}{log\left(\frac{h_1}{h_2}\right)} \approx 1 \tag{39}$$

It means that *Scheme 3* is of first-order convergence. Also, the truncation error (38) $T_{i,j} \to 0$ as $\Delta t \to 0$ and $\Delta x \to 0$ and the scheme consistent with the partial differential equation (1).

Scheme 4

Substituting $p = r = 0, q = 1 + \frac{k\Delta t}{2R}, a + b + d = 1 - \frac{k\Delta t}{2R}, a - d = \frac{v\Delta t}{R\Delta x}$ and $a + d = \frac{2D\Delta t}{R\Delta x^2} + \frac{v\Delta t}{R\Delta x}$ in (34), we get truncation error

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2}\right]_{(x_i,t_j)} + \left[\frac{k\Delta t}{2R}\frac{\partial c}{\partial t} - \frac{v\Delta x}{2R}\frac{\partial^2 c}{\partial x^2}\right]_{(x_i,t_j)} + \cdots \tag{40}$$

$$\frac{1}{\Delta t}T_{i,j} = \frac{k\Delta t}{2R}c_t - \frac{v\Delta x}{2R}c_{xx} + \cdots$$

There fore, *Scheme 4* is of first-order convergence and the scheme is consistent with the partial differential equation (1).

Semi implicit type schemes

Scheme 5

Using $p + r + q = 1,\ a + b + d = 1 - \frac{k\Delta t}{R},\ a - d = \frac{v\Delta t}{2R\Delta x},\ r - p = \frac{v\Delta t}{2R\Delta x},\ r + p = -\frac{D\Delta t}{R\Delta x^2}$ and $a + d = \frac{D\Delta t}{R\Delta x^2}$ in Eq. (34), we have that

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} + \frac{v\Delta t}{2R}\frac{\partial^2 c}{\partial x \partial t} - \frac{D\Delta t}{2R}\frac{\partial^2 c}{\partial x^2 \partial t} + \cdots\right]_{(x_i,t_j)} \tag{41}$$

$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{1}{2}c_{tt} + \frac{v}{2R}c_{xt} - \frac{D}{2R}c_{xxt}\right)\Delta t + \frac{v\Delta x^2}{6R}c_{xxx} + \cdots$$

Hence, the local truncation error is $O(\Delta t + \Delta x^2)$ when $\Delta t \to 0$ and $\Delta x \to 0$. Also, the scheme is consistent with the partial differential equation (1).

Scheme 6

Substituting $p + r + q = 1 + \frac{k\Delta t}{2R},\ a + b + d = 1 - \frac{k\Delta t}{2R},\ a - d = \frac{v\Delta t}{2R\Delta x},\ r - p = \frac{v\Delta t}{2R\Delta x},\ r + p = -\frac{D\Delta t}{R\Delta x^2}$ and $a + d = \frac{D\Delta t}{R\Delta x^2}$ in Eq. (34), we have

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{k\Delta t}{2R}\frac{\partial c}{\partial t} + \frac{v\Delta t}{2R}\frac{\partial^2 c}{\partial x \partial t} - \frac{D\Delta t}{2R}\frac{\partial^2 c}{\partial x^2 \partial t} + \cdots\right]_{(x_i,t_j)} \tag{42}$$

$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{k}{2R}c_t + \frac{v}{2R}c_{xt} - \frac{D}{2R}c_{xxt}\right)\Delta t + \frac{v\Delta x^2}{6R}c_{xxx} + \cdots$$

The scheme is consistent with the partial differential equation (1) and the local truncation error is given by $O(\Delta t + \Delta x^2)$.

Scheme 7

Using $p + q + r = 1, a + b + d = 1 - \frac{k\Delta t}{R}, a - d = \frac{v\Delta t}{2R\Delta x}, r - p = \frac{v\Delta t}{2R\Delta x}, r + p = -\frac{D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x}$ and $a + d = \frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{2R\Delta x}$ in (34), in Eq. (34), we have

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} + \frac{v\Delta t}{2R}\frac{\partial^2 c}{\partial x \partial t} - \frac{D\Delta t}{2R}\frac{\partial^2 c}{\partial x^2 \partial t} + \cdots\right]_{(x_i,t_j)} \tag{43}$$

$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{1}{2}c_{tt} + \frac{v}{2R}c_{xt} - \frac{D}{2R}c_{xxt}\right)\Delta t - \frac{v\Delta x}{2R}c_{xx} + \cdots$$

Therefore, the scheme is consistent with the partial differential equation (1) and the order of truncation error is $O(\Delta t + \Delta x)$.

Scheme 8

Using $p+q+r = 1+\frac{k\Delta t}{2R}$, $a+b+d = 1-\frac{k\Delta t}{2R}$, $a-d = \frac{v\Delta t}{2R\Delta x}$, $r-p = \frac{v\Delta t}{2R\Delta x}$, $r+p = -\frac{D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x}$ and $a+d = \frac{D\Delta t}{\Delta x^2} + \frac{v\Delta t}{2R\Delta x}$ in Eq. (34), We have that

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{k\Delta t}{2R}\frac{\partial c}{\partial t} + \frac{v\Delta t}{2R}\frac{\partial^2 c}{\partial x\partial t} - \frac{D\Delta t}{2R}\frac{\partial^2 c}{\partial x^2\partial t} + \cdots\right]_{(x_i,t_j)}$$
$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{k}{2R}c_t + \frac{v}{2R}c_{xt} - \frac{D}{2R}c_{xxt}\right)\Delta t - \frac{v\Delta x}{2R}c_{xx} + \cdots \tag{44}$$

Hence, it will be of first-order convergence. Also the scheme is consistent with the partial differential equation (1).

Implicit type schemes

Scheme 9

Substituting $p+q+r = 1$, $a = 1-\frac{k\Delta t}{R}$, $b = d = 0$, $p-r = -\frac{v\Delta t}{R\Delta x}$ and $p+r = -\frac{2D\Delta t}{R\Delta x^2}$ in Eq. (34), We get

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} + \frac{v\Delta t}{R}\frac{\partial^2 c}{\partial x\partial t} - \frac{D\Delta t}{R}\frac{\partial^2 c}{\partial x^2\partial t} + \cdots\right]_{(x_i,t_j)}$$
$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{1}{2}c_{tt} + \frac{v}{R}c_{xt} - \frac{D}{R}c_{xxt}\right)\Delta t + \frac{v\Delta x^2}{6R}c_{xxx} + \cdots \tag{45}$$

The scheme is consistent with the partial differential equation (1). If $\Delta t = \Delta x^2$, then the truncation error will be of $O(\Delta x^2)$.

Scheme 10

Using $p+q+r = 1+\frac{k\Delta t}{2R}$, $a = 1-\frac{k\Delta t}{2R}$, $b = d = 0$ $p-r = -\frac{v\Delta t}{R\Delta x}$ and $p+r = -\frac{2D\Delta t}{R\Delta x^2}$ in Eq. (34), we have that

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{k\Delta t}{2R}\frac{\partial c}{\partial t} + \frac{v\Delta t}{R}\frac{\partial^2 c}{\partial x\partial t} - \frac{D\Delta t}{R}\frac{\partial^2 c}{\partial x^2\partial t} + \cdots\right]_{(x_i,t_j)}$$
$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{k}{2R}c_t + \frac{v}{R}c_{xt} - \frac{D}{R}c_{xxt}\right)\Delta t + \frac{v\Delta x^2}{6R}c_{xxx} + \cdots \tag{46}$$

The local truncation error is $O(\Delta t + \Delta x^2)$ and the scheme is consistent with the partial differential equation (1).

Scheme 11

Substituting $p + q + r = 1, a = 1 - \frac{k\Delta t}{R}, b = d = 0, p - r = -\frac{v\Delta t}{2R\Delta x}$ and $p + r = -\frac{2D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x}$ in Eq. (34), We have that

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{\Delta t}{2}\frac{\partial^2 c}{\partial t^2} + \frac{v\Delta t}{R}\frac{\partial^2 c}{\partial x \partial t} - \frac{D\Delta t}{R}\frac{\partial^2 c}{\partial x^2 \partial t} + \cdots\right]_{(x_i,t_j)} \tag{47}$$

$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{1}{2}c_{tt} + \frac{v}{R}c_{xt} - \frac{D}{R}c_{xxt}\right)\Delta t - \frac{v\Delta x}{2R}c_{xx} + \cdots$$

Hence, the order of truncation error is $O(\Delta t + \Delta x)$. Also the scheme is consistent with the partial differential equation (1).

Scheme 12

Using $p + q + r = 1 + \frac{k\Delta t}{2R}, a = 1 - \frac{k\Delta t}{2R}, b = d = 0, p - r = -\frac{v\Delta t}{2R\Delta x}$ and $p + r = -\frac{2D\Delta t}{R\Delta x^2} - \frac{v\Delta t}{2R\Delta x}$ in Eq. (34), We have that

$$\frac{1}{\Delta t}T_{i,j} = \left[\frac{kc}{R} + \frac{\partial c}{\partial t} + \frac{v}{R}\frac{\partial c}{\partial x} - \frac{D}{R}\frac{\partial^2 c}{\partial x^2} + \frac{k\Delta t}{2R}\frac{\partial c}{\partial t} + \frac{v\Delta t}{R}\frac{\partial^2 c}{\partial x \partial t} - \frac{D\Delta t}{R}\frac{\partial^2 c}{\partial x^2 \partial t} + \cdots\right]_{(x_i,t_j)} \tag{48}$$

$$\frac{1}{\Delta t}T_{i,j} = \left(\frac{k}{2R}c_t + \frac{v}{R}c_{xt} - \frac{D}{R}c_{xxt}\right)\Delta t - \frac{v\Delta x}{2R}c_{xx} + \cdots$$

There fore, the scheme is consistent with the partial differential equation (1) and the order of truncation error is $O(\Delta t + \Delta x)$.

7 Results and Discussion

The parameters used in Cho [1], Bauer et al. [4] and Clement et al.[5] are considered for the computation of concentration of species by various numerical schemes presented in Sect. 4. The boundary conditions (2.2), (2.4) and the initial condition (2.5) with $f(t) = C_0$ (a constant dumping) are considered for the test problems. The parameter values used in computation are $C_0 = 1$ mg/l, $k = 0.01$ h^{-1}, $R = 2$, $v = 1$ cm h^{-1}, $T = 50$ h and $D = 0.18$. Analytical solution is obtained from (7).

Table 1 infers the numerical error in maximum norm obtained for various numerical schemes. It is observed that the error in central difference schemes 2, 6, and 10 increases compare to schemes 1, 5, and 9, respectively. The reason for this is that the source term (C_{avg}) in (9) is approximated by C_P^n in odd-numbered schemes 1, 3, 5, 7, 9, and 11, while the same source term is approximated by $\frac{C_P^n + C_P^{n+1}}{2}$ (i.e., average

Table 1 Numerical error

Scheme	L_∞ error $h_1 = 0.3, h_2 = 0.2, h_3 = 0.1$			Order of convergence	
Central	$\|c - C_{h_1}\|_\infty$	$\|c - C_{h_2}\|_\infty$	$\|c - C_{h_3}\|_\infty$	$log\frac{N_1}{N_2}/log\frac{h_1}{h_2}$	$log\frac{N_2}{N_2}/log\frac{h_2}{h_3}$
Scheme 1	0.0151839	0.0065515	0.0016103	2.0730307	2.0244959
Scheme 2	0.0156539	0.0067565	0.0016613	2.0722254	2.0239634
Scheme 5	0.0037391	0.0016503	0.0004113	2.0171596	2.0044653
Scheme 6	0.0043201	0.0019093	0.0004753	2.0138400	2.0061335
Scheme 9	0.0126231	0.0058558	0.0015083	1.8943574	1.9569428
Scheme 10	0.0130631	0.0059716	0.0015196	1.9305645	1.9744258
Upwind	L_∞ error $h_1 = 1, h_2 = 0.5, h_3 = 0.4$			Order of convergence	
Scheme 3	0.0879704	0.0541474	0.0454174	0.7001266	0.7878945
Scheme 4	0.0844378	0.0520764	0.0437294	0.6972593	0.7828649
Scheme 7	0.1459378	0.0958983	0.0823154	0.6057765	0.6844476
Scheme 8	0.1429908	0.0941353	0.0808434	0.6031146	0.6821581
Scheme 11	0.1632868	0.1150218	0.1005767	0.5055008	0.6014114
Scheme 12	0.1606958	0.1135018	0.0992857	0.5016170	0.5996907

where $N_1 = \|c - C_{h_1}\|_\infty$, $N_2 = \|c - C_{h_2}\|_\infty$ and $N_3 = \|c - C_{h_3}\|_\infty$
Central difference: $\Delta t = h^2$ and Upwind: $\Delta t = h$

of C_P taken over n and $n + 1$ time levels) in even-numbered schemes 2, 4, 6, 8, 10, and 12. In the similar manner, the error in upwind schemes 4, 8, and 12 decreases compare to upwind schemes 3, 7, and 11, respectively. Hence, averaging the source term C_{avg} in (9) at n and $n + 1$ time level is a good technique for upwind schemes and a bad choice for central difference schemes.

It is also observed that the implicit type schemes 5, 6, 9, and 10 yield better result in comparing with explicit nature schemes 1 and 2 as far as central difference schemes are concerned, but there is a reverse phenomenon in upwind schemes. That is, the explicit upwind schemes 3 and 4 give better result in comparing with implicit nature upwind schemes 7, 8, 11, and 12.

Theoretically, second- and first-order convergences are obtained for central difference and upwind schemes, respectively. This is validated numerically which can be seen from Table 1. Further, the explicit upwind schemes 3 and 4 converge much faster than implicit nature upwind schemes 7, 8, 11, and 12. Thus, the averaging technique for reaction (i.e., source) term and upwinding for the advection term play a crucial role in numerical schemes for advecton–diffusion–reaction problems.

Table 2 is the summarization of theoretical results from Sects. 5 and 6. In general, explicit and implicit nature schemes are, respectively, conditionally and unconditionally stable for time-dependent problems in the absence of reaction (i.e., source) term. From Table 2, it is clear that the implicit nature schemes 5, 7, 9, and 11 are conditionally stable, while other implicit nature numerical schemes 6, 8, 10, and 12

Table 2 Summary of stability condition and order of convergence from theoretical results obtained from Sects. 5 and 6

Scheme	Stability condition	Order of error
Scheme 1	$\Delta t \leq \frac{R(8D+2k\Delta x^2)\Delta x^2}{16D^2+k^2\Delta x^4+8Dk\Delta x^2}$ $\frac{v\Delta x}{D} \leq 2, \frac{k\Delta t}{R} \leq 1$	Second
Scheme 2	$\Delta t \leq \frac{R(8D+4k\Delta x^2)\Delta x^2}{16D^2+8Dk\Delta x^2}$ $\frac{v\Delta x}{D} \leq 2, \frac{k\Delta t}{R} \leq 2$	Second
Scheme 3	$\Delta t \leq \frac{R(8D+4v\Delta x+2k\Delta x^2)\Delta x^2}{16D^2+16Dv\Delta x+8Dk\Delta x^2+4vk\Delta x^3+4v^2\Delta x^2+k^2\Delta x^4}$ $\frac{k\Delta t}{R} \leq 1$	First
Scheme 4	$\Delta t \leq \frac{R(8D+4v\Delta x+4k\Delta x^2)\Delta x^2}{16D^2+16Dv\Delta x+8Dk\Delta x^2+4vk\Delta x^3+4v^2\Delta x^2}$ $\frac{k\Delta t}{R} \leq 2$	First
Scheme 5	$\frac{k\Delta t}{R} \leq 2$	Second
Scheme 6	Unconditionally stable	Second
Scheme 7	$\frac{k\Delta t}{R} \leq 2$	First
Scheme 8	Unconditionally stable	First
Scheme 9	$\frac{k\Delta t}{R} \leq 2$	Second
Scheme 10	Unconditionally stable	Second
Scheme 11	$\frac{k\Delta t}{R} \leq 2$	First
Scheme 12	Unconditionally stable	First

are unconditionally stable for the advection-diffusion–reaction equation (1). This is due to the fact that, the reaction (i.e., source) term (C_{avg}) in (9) in schemes 6, 8, 10, and 12 is approximated by $\frac{C_P^n+C_P^{n+1}}{2}$, while the same term in schemes 5, 7, 9, and 11 is approximated by C_P^n.

References

1. Cho, C.M.: Convective transport of ammonium with nitrification in soil. Can. J. Soil Sci. **51**, 339–350 (1971)
2. Sun, Y., Clement, T.P.: A generalized decomposition method for solving coupled multi-species reactive transport problems. Transp. Porous Media **37**, 327–346 (1999)
3. Sun, Y., Petersen, J.N., Clement, T.P., Skeen, R.S.: Development of analytical solutions for multispecies transport with serial and parallel reactions. Water Resour. Res. **35**, 185–190 (1999)
4. Bauer, P., Attinger, S., Kinzelbach, W.: Transport of decay chain in homogeneous porous media: analytical solutions. J. Contam. Hydrol. **49**, 217–239 (2001)
5. Clement, T.P., Quezada, C.R., Lee, K.-K.: Generalised solution to multi-dimensional multi species transport equations coupled with a first-order reaction network involving distinct retardation factors. Adv. Water Resour. **27**, 507–520 (2004)

6. Clement, T.P.: A modular computer model for simulating reactive multi species transport in three dimensional groundwater systems. Technical Report, Pacific Northwest National Laboratory, Richland, Washington, PNNL-SA-28967 (1997)
7. Clement, T.P., Johnson, C.D., Sun, Y., Klecka, G.M., Bartlett, C.: Natural attenuation of chlorinated solvent compounds: model development and field-scale application at the Dover site. J. Contam. Hydrol. **42**, 113–140 (2000)
8. Clement, T.P., Sun, Y., Hooker, B.S., Petersen, J.N.: Modeling multispecies reactive transport in groundwater aquifers. Groundw. Monit. Remediat. **18**(2), 79–92 (1998)
9. Van Genutchen, M.T.: Convective-dispersive transport of solutes involved in sequential first-order decay reactions. Comput. Geosci. **11**, 129–147 (1985)
10. Elango, L., Brindha, K., Kalpana, L., Sunny, F., Nair, R.N., Murugan, R.: Groundwater flow and radionuclide decay-chain transport modelling around a proposed uranium tailings pond in India. Hydrogeol. J. (2012)
11. Smith, S.D.: Numerical Solutions of Partial Differential Equations: Finite Difference Methods. Oxford University Press (1985)