Total Variation Diminishing Finite Volume Scheme for Multi Dimensional Multi Species Transport with First Order Reaction Network

S. Prabhakaran and L. Jones Tarcius Doss

Abstract A Total Variation Diminishing (TVD) scheme for multi-species transport with first-order reaction network in multidimensional space is discussed in this article. The partial differential equations which describe this multi-species transport with chain reactions are in the form of a coupled system. This system is then solved by the TVD scheme with various flux limiters. The numerical diffusion controlled by the flux limiters is explained in detail. The stability and consistency conditions of the TVD scheme is also derived. The relation between the flux limiters and mesh parameters is obtained through stability conditions. A necessary condition for a scheme to be TVD is also derived.

Keywords Total variation diminishing · Finite volume method · Contamination transport · Stability · Consistency · Flux limiters

1 Introduction

Groundwater pollution attracted researchers for evaluating the movement of degradable contents in the groundwater system. The transport of these degradable species is governed by advection-diffusion–reaction (ADR) equation. Several researchers have developed an analytical solution for the species transport equation. van Genutchen [1] has given a complete review on analytical solution for one-dimensional advection–diffusion equation under various initial and boundary conditions. Domenico [2] has derived an analytical solution for multidimensional single species transport. Cho [3] has provided an analytical solution for one- dimensional three species transport. Bauer et al. [4], Clement et al. [5–7], and Sun et al. [8, 9] have discussed various

S. Prabhakaran (✉)
Department of Mathematics with Computer Applications, PSG College of Arts & Science, Civil Aerodrome, Coimbatore 641014, India
e-mail: karan.shivam@gmail.com

L. Jones Tarcius Doss
Department of Mathematics, Anna University, Chennai 600025, India

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models with analytical solutions for multi-species transport in multi-dimensions. The limitations in deriving an analytical solution and the development of modern sophisticated computing machines lead to serious research on numerical techniques.

Finite difference methods are popular among researchers in earlier days. Sheu et al. [10] and Calvo et al. [11] have used finite difference method for ADR equation. Hundsdorfer et al. [12] have presented a review of ADR equations mostly focusing on finite difference methods. Sibert et al. [13] has modeled fish movement using one-dimensional ADR equation and solved numerically using the finite difference method. The search for providing continuous solution to this problem landed with finite element methods. Houston et al. [14] has used the hp-finite element method for providing a solution to the ADR equation. Ayuso and Donatella Marini [15], Ern et al. [16] and Georgoulis et al. [17] have made contribution to a solution for the same using discontinuous Galerkin method. Idelsohn et al. [18] have applied Petrov-Galerkin method on the ADR equation. Most recently, Mudunuru and Nakshatrala [19] have used a finite element method for solving the ADR equation by enforcing maximum principle with the concern on element-wise species balance.

Finite volume method (FVM) is one of the handy tools for researchers in computational fluid dynamics in recent days due to the property of preservation of exact mass conservation in the local control volume. Eymard et al. [20] have given a comprehensive study on finite volume methods in his monograph. LeVeque [21] has discussed finite volume methods in his book on hyperbolic problems with engineering applications. Ramos [22] has solved reaction–diffusion problem using the finite volume method. Arachchige and Pettet [23] has used FVM for solving ADR equation with linearization in the time domain. ten Thije Boonkkamp and Anthonissen [24] have used a finite volume-complete flux scheme for solving ADR equations. Upwind finite volume schemes have become very popular among researchers due to their advantage over capturing flow direction. The disadvantage of the upwind technique is numerical diffusion. Several searchers tried to control this artificial diffusion and brought it up with Total Variation Diminishing technique (TVD). A concept of flux limiter is introduced in TVD schemes. van Leer [25] is one of the pioneers of this concept. Sweby [26] and Harten [27, 28] have used TVD scheme for solving one-dimensional transport equation. In fact, Sweby has given sufficient conditions for a scheme to be TVD. Jameson and Lax [29] have derived abstract conditions for the construction of total variation diminishing difference schemes. Shu [30] has used Runge–Kutta-type TVD time discretization for transport equation. Thereafter, several researches have been done on TVD schemes.

The governing equation for transport of species with first-order reaction network with liquid phase degradation is given by the following system of advection–diffusion reaction equations [6]:

$$R_k \frac{\partial U_k}{\partial t} - \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(D_i \frac{\partial U_k}{\partial x_i}\right) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(v_i U_k) = \sum_{d=1}^{k-1} Y_{k/d} K_d U_d - K_k U_k + \sum_{d=k+1}^{r} Y_{k/d} K_d U_d, \quad k = 1, 2, 3..., r \tag{1}$$

where n is the total number of species; U_k the concentration of kth species $[ML^{-3}]$; D_i the dispersion coefficient $[L^2T^{-1}]$; v_i the transport velocity $[LT^{-1}]$; K_k the first-order contaminant destruction rate constant of k^{th} species $[T^{-1}]$; R_k the retardation coefficient, and $Y_{k/d}$ the effective yield factor that describes the mass of a species k produced from another species d $[MM^{-1}]$. The kinetics of reaction is assumed to be of first order. The concentration of kth species U_k $(k = 1, 2, ..., r)$ in the first-order reaction network is to be determined for three-dimensional flow at $X_P = (x_1, x_2, x_3)$ at any given time t.

In case of degradation process occurs in both solid and liquid phase, then the governing equation is given by

$$R_k \frac{\partial U_k}{\partial t} - \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(D_i \frac{\partial U_k}{\partial x_i}\right) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(v_i U_k) = \sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_d - R_k K_k U_k + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_d \quad k = 1, 2, 3..., r \tag{2}$$

The difference between Eqs. (1) and (2) lies in the presence of retardation factor R_k in the reaction term of 2.

2 Numerical Approximation

Let us discuss a control volume before deriving numerical approximation. The letters E, W, N, S, T, and B in the control volume represent east, west, north, south, top, and bottom nodal points located at the middle of their respective sides in the outer cube, respectively. A numerical solution is obtained at the nodal point (P) located at the centroid of the cube. Similarly, the letters e, w, n, s, t_p, and b represent east, west, north, south, top and bottom faces of the inner cube. Spatial step size is the difference between the nodal points. Faces of the control volume are located half-way between nodes. The vector form of a governing equation (2) can be written as

$$R_k \frac{\partial U_k}{\partial t} - \overline{\nabla} \cdot (\overline{\nabla} D U_k) + \overline{\nabla} \cdot (v U_k) = \sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_d - R_k K_k U_k + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_d, \tag{3}$$

where $\overline{\nabla} D U_k = (D_1 \frac{\partial U_k}{\partial x_1}, D_2 \frac{\partial U_k}{\partial x_2}, D_3 \frac{\partial U_k}{\partial x_3})$ and $v U_k = (v_1 U_k, v_2 U_k, v_3 U_k)$. Integrating the above equation first with respect to time from t_m to $t_m + \Delta t = t_{m+1}$ and then integrating over a local control volume CV [31], we obtain the following:

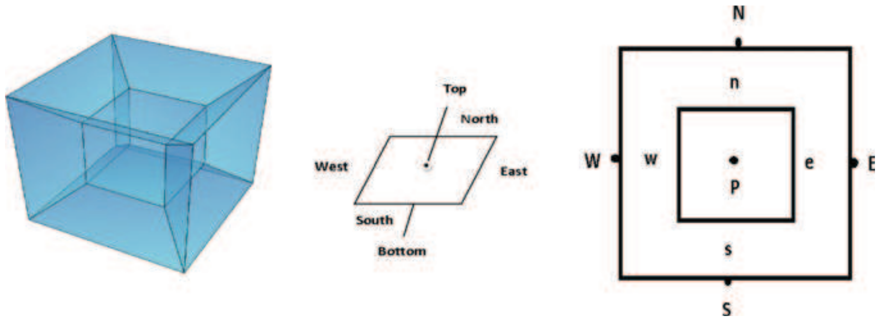

Fig. 1 3D control volume

$$R_k \int_{CV} \int_{t_m}^{t_{m+1}} \frac{\partial U_k}{\partial t} dt dV = \int_{CV} \int_{t_m}^{t_{m+1}} \overline{\nabla} \cdot (\overline{\nabla} D U_k) dt dV - \int_{CV} \int_{t_m}^{t_{m+1}} \overline{\nabla} \cdot (v U_k) dt dV$$
$$+ \int_{CV} \int_{t_m}^{t_{m+1}} \left(\sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_d - R_k K_k U_k + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_d \right) dt dV.$$

Using forward Euler for time integration, we obtain

$$R_k \int_{CV} (U_k^{m+1} - U_k^m) dV = \Delta t \int_{CV} \overline{\nabla} \cdot (\overline{\nabla} D U_k^m) dV - \Delta t \int_{CV} \overline{\nabla} \cdot (v U_k^m) dV$$
$$+ \Delta t \int_{CV} \left(\sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_d^m - R_k K_k U_k^m + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_d^m \right) dV.$$

The first two volume integrals over CV on the right-hand side can be converted into surface integral by applying the Gauss divergence theorem as follows:

$$R_k \int_{CV} (U_k^{m+1} - U_k^m) dV = \Delta t \int_A \overrightarrow{n} . \overline{\nabla} D U_k^m dA - \Delta t \int_A \overrightarrow{n} \cdot (v U_k^m) dA$$
$$- \Delta t \int_{CV} R_k K_k U_k^m dV + \Delta t \int_{CV} \sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_d^m dV$$
$$+ \Delta t \int_{CV} \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_d^m dV,$$

where $\overrightarrow{n}$ is the unit outward normal to the surface A of a control volume. The surface integral can be split into six surfaces (S), namely east (e), west (w), north (n), south (s), top (t_p), and bottom (b) as follows:

$$R_k \quad \int_{CV} (U_k^{m+1} - U_k^m) dV = \Delta t \sum \int_S \overrightarrow{n} \cdot \overline{\nabla} D U_k^m dS - \Delta t \sum \int_S \overrightarrow{n} \cdot (v U_k^m) dS$$
$$+ \Delta t \int_{CV} \left(\sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_d^m - R_k K_k U_k^m + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_d^m \right) dV.$$

$$R_k \int_{CV} (U_k^{m+1} - U_k^m) dV = \Delta t \left[A_e \left(D_1 \frac{\partial U_k^m}{\partial x_1} \right)_e - A_w \left(D_1 \frac{\partial U_k^m}{\partial x_1} \right)_w + A_n \left(D_2 \frac{\partial U_k^m}{\partial x_2} \right)_n \right.$$
$$\left. - A_s \left(D_2 \frac{\partial U_k^m}{\partial x_2} \right)_s + A_{t_p} \left(D_3 \frac{\partial U_k^m}{\partial x_3} \right)_{t_p} - A_b \left(D_3 \frac{\partial U_k^m}{\partial x_3} \right)_b \right] - \Delta t \left[A_e (v_1 U_k^m)_e \right.$$
$$\left. - A_w (v_1 U_k^m)_w + A_n (v_2 U_k^m)_n - A_s (v_2 U_k^m)_s + A_{t_p} (v_3 U_k^m)_{t_p} - A_b (v_3 U_k^m)_b \right]$$
$$+ \Delta t \int_{CV} \left(\sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_d^m - R_k K_k U_k^m + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_d^m \right) dV,$$

where $A_e = A_w = \Delta x_2 \Delta x_3$, $A_n = A_s = \Delta x_1 \Delta x_3$ and $A_{t_p} = A_b = \Delta x_1 \Delta x_2$. Let us assume that the control volume is fixed for all time. Taking the average over a control volume at the centroid P for left- and right-hand side integrals, we obtain the following:

$$R_k (U_{kP}^{m+1} - U_{kP}^m) \int_{CV} dV = \Delta t \left[A_e D_1 \left(\frac{\partial U_k^m}{\partial x_1} \right)_e - A_w D_1 \left(\frac{\partial U_k^m}{\partial x_1} \right)_w + A_n D_2 \left(\frac{\partial U_k^m}{\partial x_2} \right)_n \right]$$
$$+ \Delta t \left[- A_s D_2 \left(\frac{\partial U_k^m}{\partial x_2} \right)_s + A_{t_p} D_3 \left(\frac{\partial U_k^m}{\partial x_3} \right)_{t_p} - A_b D_3 \left(\frac{\partial U_k^m}{\partial x_3} \right)_b \right]$$
$$- \Delta t \left[A_e v_1 U_{ke}^m - A_w v_1 U_{kw}^m + A_n v_2 U_{kn}^m - A_s v_2 U_{ks}^m + A_{t_p} v_3 U_{kt_p}^m - A_b v_3 U_{kb}^m \right]$$
$$+ \Delta t \left(\sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_{dP}^m - R_k K_k U_{kP}^m + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_{dP}^m \right) \int_{CV} dV,$$

where U_{kP} is average taken over a control volume and $\int_{CV} dV = \Delta V = \Delta x_1 \Delta x_2 \Delta x_3$. Let us apply central difference for the terms $\frac{\partial U_k^m}{\partial x_1}$, $\frac{\partial U_k^m}{\partial x_2}$, $\frac{\partial U_k^m}{\partial x_3}$ and bringing $R_k \Delta V$ term to the right- hand side, we obtain

$$U_{kP}^{m+1} - U_{kP}^m = \left[\frac{D_1 \Delta t}{R_k \Delta x_1^2} \left(U_{kW}^m - 2U_{kP}^m + U_{kE}^m \right) + \frac{D_2 \Delta t}{R_k \Delta x_2^2} \left(U_{kS}^m - 2U_{kP}^m + U_{kN}^m \right) \right.$$
$$\left. + \frac{D_3 \Delta t}{R_k \Delta x_3^2} \left(U_{kB}^m - 2U_{kP}^m + U_{kT}^m \right) \right] + \left[- \frac{v_1 \Delta t}{R_k \Delta x_1} U_{ke}^m - \frac{v_2 \Delta t}{R_k \Delta x_2} U_{kn}^m - \frac{v_3 \Delta t}{R_k \Delta x_3} U_{kt_p}^m \right.$$
$$\left. + \frac{v_1 \Delta t}{R_k \Delta x_1} U_{kw}^m + \frac{v_2 \Delta t}{R_k \Delta x_2} U_{ks}^m + \frac{v_3 \Delta t}{R_k \Delta x_3} U_{kb}^m \right]$$
$$+ \left[\left(\sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_{dP}^m - R_k K_k U_{kP}^m + \sum_{d=k+1}^{r} R_d Y_{k/d} K_d U_{dP}^m \right) \frac{\Delta t}{R_k} \right]. \quad (4)$$

The approximation for advection term (that is, second term on right-hand side) is derived by using slope reconstruction technique. Expanding U_{ke}^m in Taylor's series and truncating after second term in x_1 direction, we have

$$U_{ke}^m \approx U_{kP}^m + \frac{\Delta x_1}{2}\left(\frac{\partial U_k^m}{\partial x_1}\right)_P.$$

The flux term $\frac{\partial U_k^m}{\partial x_1}$ in above is called anti-diffusion term. It controls the numerical diffusion. This has been explained in Sect. 4. Introducing flux limiter $\psi(r)$ to control anti-diffusion and using forward difference approximation for flux term, we obtain

$$U_{ke}^m \approx U_{kP}^m + \frac{\psi(r_e)}{2}(U_{kE}^m - U_{kP}^m) \quad \text{where} \quad r_e = \frac{U_{kP}^m - U_{kW}^m}{U_{kE}^m - U_{kP}^m}.$$

Flux limiters for all other directions can be obtained in a similar way,

$$U_{kw}^m \approx U_{kW}^m + \frac{\psi(r_w)}{2}(U_{kP}^m - U_{kW}^m) \quad \text{where} \quad r_w = \frac{U_{kW}^m - U_{kWW}^m}{U_{kP}^m - U_{kW}^m};$$
$$U_{kn}^m \approx U_{kP}^m + \frac{\psi(r_n)}{2}(U_{kN}^m - U_{kP}^m) \quad \text{where} \quad r_n = \frac{U_{kP}^m - U_{kS}^m}{U_{kN}^m - U_{kP}^m};$$
$$U_{ks}^m \approx U_{kS}^m + \frac{\psi(r_s)}{2}(U_{kP}^m - U_{kS}^m) \quad \text{where} \quad r_s = \frac{U_{kS}^m - U_{kSS}^m}{U_{kP}^m - U_{kS}^m};$$
$$U_{kt_p^m} \approx U_{kP}^m + \frac{\psi(r_{t_p})}{2}(U_{kT}^m - U_{kP}^m) \quad \text{where} \quad r_{t_p} = \frac{U_{kP}^m - U_{kB}^m}{U_{kT}^m - U_{kP}^m};$$
and $U_{kb}^m \approx U_{kB}^m + \frac{\psi(r_b)}{2}(U_{kP}^m - U_{kB}^m) \quad \text{where} \quad r_b = \frac{U_{kB}^m - U_{kBB}^m}{U_{kP}^m - U_{kB}^m}.$

Substituting the above in (4), we obtain

$$\begin{aligned} U_{kP}^{m+1} &= A_P U_{kP}^m + A_W U_{kW}^m + A_E U_{kE}^m + A_S U_{kS}^m + A_N U_{kN}^m + A_B U_{kB}^m + A_T U_{kT}^m \\ &\quad + \left(\sum_{d=1}^{k-1} c_d U_{dP}^m + \sum_{d=k+1}^{n_1} c_d U_{dP}^m\right)\frac{\Delta t}{R_k}, \end{aligned} \tag{5}$$

where

$A_P = 1 - \frac{2D_1\Delta t}{R_k\Delta x_1^2} - \frac{2D_2\Delta t}{R_k\Delta x_2^2} - \frac{2D_3\Delta t}{R_k\Delta x_3^2} - \frac{v_1\Delta t}{R_k\Delta x_1} - \frac{v_2\Delta t}{R_k\Delta x_2} - \frac{v_3\Delta t}{R_k\Delta x_3} + \frac{v_1\Delta t}{2R_k\Delta x_1}$
$[\psi(r_e) + \psi(r_w)] + \frac{v_2\Delta t}{2R_k\Delta x_2}[\psi(r_s) + \psi(r_n)] + \frac{v_3\Delta t}{2R_k\Delta x_3}[\psi(r_{t_p}) + \psi(r_b)] - K_k\Delta t$,
$A_W = \frac{D_1\Delta t}{R_k\Delta x_1^2} + \frac{v_1\Delta t}{R_k\Delta x_1} - \frac{v_1\Delta t}{2R_k\Delta x_1}\psi(r_w)$, $A_E = \frac{D_1\Delta t}{R_k\Delta x_1^2} - \frac{v_1\Delta t}{2R_k\Delta x_1}\psi(r_e)$,
$A_N = \frac{D_2\Delta t}{R_k\Delta x_2^2} - \frac{v_2\Delta t}{2R_k\Delta x_2}\psi(r_n)$, $A_S = \frac{D_2\Delta t}{R_k\Delta x_2^2} + \frac{v_2\Delta t}{R_k\Delta x_2} - \frac{v_2\Delta t}{2R_k\Delta x_2}\psi(r_s)$,
$A_T = \frac{D_3\Delta t}{R_k\Delta x_3^2} - \frac{v_3\Delta t}{2R_k\Delta x_3}\psi(r_{t_p})$, $A_B = \frac{D_3\Delta t}{R_k\Delta x_3^2} + \frac{v_3\Delta t}{R_k\Delta x_3} - \frac{v_3\Delta t}{2R_k\Delta x_3}\psi(r_b)$ and
$c_d = R_d Y_{k/d} K_d$.

Table 1 List of flux limiters

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	$Max[0, Min(2r, (3 + r)/4, (1 + 3r)/4, 2)]$		

3 Stability Analysis

Let us discuss the stability of the proposed scheme in this section. The general form of explicit scheme for three dimensional is given by $U_{kP}^{m+1} = A_P U_{kP}^m + A_E U_{kE}^m + A_W U_{kW}^m + A_N U_{kN}^m + A_S U_{kS}^m + A_T U_{kT}^m + A_B U_{kB}^m$. The stability condition for this scheme is derived.

Theorem 1
Let $U_{kP}^{m+1} = A_P U_{kP}^m + A_E U_{kE}^m + A_W U_{kW}^m + A_N U_{kN}^m + A_S U_{kS}^m + A_T U_{kT}^m + A_B U_{kB}^m$ *be the general form of explicit finite difference scheme for any linear time-dependent partial differential equation in three dimensions with equal mesh length and mesh points in spatial directions. If the coefficients* $A_P \geq 0, A_W \geq 0, A_E \geq 0, A_N \geq 0, A_S \geq 0, A_T \geq 0$ *and* $A_B \geq 0$ *and satisfy* $(A_P + A_E + A_W + A_N + A_S + A_T + A_B)^2 \leq 1 + 4A_P(A_E + A_W + A_N + A_S + A_T + A_B)$*, then the scheme is stable.*

Proof
Consider the general form of explicit scheme

$$U_{kP}^{m+1} = A_P U_{kP}^m + A_E U_{kE}^m + A_W U_{kW}^m + A_N U_{kN}^m + A_S U_{kS}^m + A_T U_{kT}^m + A_B U_{kB}^m \tag{6}$$

with A_P, A_W, A_E, A_N, A_S, A_T and A_B are greater than or equal to zero. Substituting $U_{kP}^m = B\xi^m e^{i\alpha\theta_1} e^{i\beta\theta_2} e^{i\gamma\theta_3}$ in above explicit scheme, we have

$$\begin{aligned}\xi &= A_P + (A_E + A_W)\cos\theta_1 + (A_N + A_S)\cos\theta_2 + (A_T + A_B)\cos\theta_3 \\ &\quad + i(A_E - A_W)\sin\theta_1 + i(A_N - A_S)\sin\theta_2 + i(A_T - A_B)\sin\theta_3).\end{aligned}$$

von Neumann criteria for stability is given by $|\xi| \leq 1$ which implies $|\xi|^2 \leq 1$. We therefore have that

$$\begin{aligned}&|A_P + (A_E + A_W)\cos\theta_1 + (A_N + A_S)\cos\theta_2 + (A_T + A_B)\cos\theta_3 \\ &+i(A_E - A_W)\sin\theta_1 + i(A_N - A_S)\sin\theta_2 + i(A_T - A_B)\sin\theta_3)|^2 \leq 1.\end{aligned}$$

Let us assume that $\theta_1 = \theta_2 = \theta_3 = \theta$. That is, the number of nodal points in all directions are equal with the same mesh length. Then, we have

$$
\begin{aligned}
|A_P + (A_E + A_W + A_N + A_S + A_T + A_B)\cos\theta \\
+ i(A_E - A_W + A_N - A_S + A_T - A_B)\sin\theta)|^2 &\le 1; \\
A_P^2 + (A_E + A_W + A_N + A_S + A_T + A_B)^2\cos^2\theta \\
+ 2A_P(A_E + A_W + A_N + A_S + A_T + A_B)\cos\theta \\
+ (A_E - A_W + A_N - A_S + A_T - A_B)^2\sin^2\theta &\le 1; \\
A_P^2 + A_E^2 + A_W^2 + A_N^2 + A_S^2 \\
+ A_T^2 + A_B^2 + 2(A_E A_W + A_N A_S + A_T A_B)(\cos^2\theta - \sin^2\theta) \\
+ 2A_P(A_E + A_W + A_N + A_S + A_T + A_B)\cos\theta &\le 1; \\
(A_P + A_E + A_W + A_N + A_S + A_T + A_B)^2 \\
- 2A_P(A_E + A_W + A_N + A_S + A_T + A_B)(1 - \cos\theta) \\
- 2(A_E A_W + A_N A_S + A_T A_B)(1 - \cos 2\theta) &\le 1;
\end{aligned}
$$

$$
\begin{aligned}
(A_P + A_E + A_W + A_N + A_S + A_T + A_B)^2 &\le 1 + 4(A_E A_W + A_N A_S + A_T A_B)\sin^2\theta \\
&\quad + 4A_P(A_E + A_W + A_N + A_S + A_T + A_B)\sin^2\frac{\theta}{2}; \\
(A_P + A_E + A_W + A_N + A_S + A_T + A_B)^2 &\le 1 + 16(A_E A_W + A_N A_S + A_T A_B)\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2} \\
&\quad + 4A_P(A_E + A_W + A_N + A_S + A_T + A_B)\sin^2\frac{\theta}{2}; \\
(A_P + A_E + A_W + A_N + A_S + A_T + A_B)^2 \\
16(A_E A_W + A_N A_S + A_T A_B)\sin^4\frac{\theta}{2} &\le 1 + 16(A_E A_W + A_N A_S + A_T A_B)\sin^2\frac{\theta}{2} \\
&\quad + 4A_P(A_E + A_W + A_N + A_S + A_T + A_B)\sin^2\frac{\theta}{2}.
\end{aligned}
$$

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

$$
(A_P + A_E + A_W + A_N + A_S + A_T + A_B)^2 \le 1 + 4A_P(A_E + A_W + A_N + A_S + A_T + A_B). \tag{7}
$$

Therefore, any numerical scheme satisfying (7) and positivity on coefficients is stable.

The summation terms $(\sum_{d=1}^{k-1} c_d U_{dP}^m + \sum_{d=k+1}^{n} c_d U_{dP}^m)\frac{\Delta t}{R_k}$ in (5) constitute other species transport except the current species k. Further, c_d, R_k and Δt are all positive. The stability of entire k species depends on the stability of each species transport in the network. Therefore, it is enough to demonstrate the stability of each species transport on the assumption of the other $k-1$ species having stable value. Hence, the stability of a system in (5) depends on the stability of the following for each k

$$
U_{kP}^{m+1} = A_P U_{kP}^m + A_E U_{kE}^m + A_W U_{kW}^m + A_N U_{kN}^m + A_S U_{kS}^m + A_T U_{kT}^m + A_B U_{kB}^m. \tag{8}
$$

The stability condition (7) is derived for equal mesh size in spatial directions. Let us assume that $\Delta x = \Delta x_1 = \Delta x_2 = \Delta x_3$. Further, the value of ψ varies over spatial and temporal directions. Therefore, a general function $\psi(r)$ is considered for stability analysis and truncation error. Substituting the coefficients $A_P, A_E, A_W, A_S, A_N, A_T$, and A_B in (7) with these assumptions, the following stability condition is obtained for (8) and hence for (5)

$$\Delta t \leq \frac{\frac{2D}{R_k \Delta x^2} + \frac{v}{R_k \Delta x} - \frac{v}{R_k \Delta x}\psi(r) + \frac{K_k}{2}}{\frac{4D^2}{R_k^2 \Delta x^4} + \frac{4Dv}{R_k^2 \Delta x^3} + \frac{v^2}{R_k^2 \Delta x^2} + \frac{2DK_k}{R_k \Delta x^2} + \frac{vK_k}{R_k \Delta x} + \frac{K_k^2}{4} - \left[\frac{2v^2}{R_k^2 \Delta x^2} + \frac{4Dv}{R_k^2 \Delta x^3} + \frac{vK_k}{R_k \Delta x}\right]\psi(r) + \frac{v^2}{R_k^2 \Delta x^2}\psi(r)^2} \tag{9}$$

where $D = D_1 + D_2 + D_3$ and $v = v_1 + v_2 + v_3$. The condition on the flux limiter for the total variation diminishing is $0 \leq \psi(r) \leq 2$. Therefore, the stability condition in (9) must satisfy for the least value of $\psi(r)$ (that is, $\psi(r) = 0$). Hence, we get

$$\Delta t_1 \leq \frac{\frac{2D}{R_k \Delta x^2} + \frac{v}{R_k \Delta x} + \frac{K_k}{2}}{\frac{4D^2}{R_k^2 \Delta x^4} + \frac{4Dv}{R_k^2 \Delta x^3} + \frac{v^2}{R_k^2 \Delta x^2} + \frac{2DK_k}{R_k \Delta x^2} + \frac{vK_k}{R_k \Delta x} + \frac{K_k^2}{4}} \tag{10}$$

The stability condition in (9) must also satisfy for the maximum value of $\psi(r)$ (that is, $\psi(r) = 2$).

$$\Delta t_2 \leq \frac{\frac{2D}{R_k \Delta x^2} - \frac{v}{R_k \Delta x} + \frac{K_k}{2}}{\frac{4D^2}{R_k^2 \Delta x^4} - \frac{4Dv}{R_k^2 \Delta x^3} + \frac{v^2}{R_k^2 \Delta x^2} + \frac{2DK_k}{R_k \Delta x^2} - \frac{vK_k}{R_k \Delta x} + \frac{K_k^2}{4}} \tag{11}$$

The above is the relation between spatial step size and temporal step size for stable TVD schemes. Choose always $\Delta t \leq Min(\Delta t_1, \Delta t_2)$ to get a stable scheme.

4 Truncation Error and Consistency

The truncation error for an explicit numerical scheme at interior nodal point (X_P, t_m) is defined by Smith [32]

$$T_{P,m} = \frac{1}{\Delta t}\left[U_k(X_P, t_{m+1}) - U_{kP}^{m+1}\right],$$

where $U_k(X_P, t_{m+1})$ and U_{kP}^{m+1} are the values of exact and numerical solution of kth species U_k at (X_P, t_{m+1}), respectively. From (5)

$$\Delta t T_{P,m} = U_k(X_P, t_{m+1}) - A_P U_{kP}^m - A_E U_{kE}^m - A_W U_{kW}^m - A_N U_{kN}^m - A_S U_{kS}^m - A_T U_{kT}^m - A_B U_{kB}^m - \left(\sum_{d=1}^{k-1} c_d U_{dP}^m + \sum_{d=k+1}^{n} c_d U_{dP}^m\right)\frac{\Delta t}{R_k}.$$

The truncation error for explicit numerical scheme can be obtained by replacing numerical solution with exact solution. Thus, we have

$$\begin{aligned}\Delta t T_{P,m} &= U_k(X_P, t_{m+1}) - A_P U_k(X_P, t_m) - A_E U_k(X_E, t_m) - A_W U_k(X_W, t_m) \\ &- A_N U_k(X_N, t_m) - A_S U_k(X_S, t_m) - A_T U_k(X_T, t_n) - A_B U_k(X_B, t_n) \\ &- \left(\sum_{d=1}^{k-1} c_d U_k(X_P, t_m) + \sum_{d=k+1}^{n} c_d U_k(X_P, t_m)\right)\frac{\Delta t}{R_k}.\end{aligned}$$

Expanding the above using Taylor series, we obtain that

$$\begin{aligned}\Delta t T_{P,m} &= \left[U_{kP}^m + \Delta t\frac{\partial U_{kP}^m}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 U_{kP}^m}{\partial t^2} + ...\right] - A_P U_{kP}^m \\ &- A_E\left[U_{kP}^m + \Delta x_1\frac{\partial U_{kP}^m}{\partial x_1} + \frac{\Delta x_1^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_1^2} + ...\right] \\ &- A_W\left[U_{kP}^m - \Delta x_1\frac{\partial U_{kP}^m}{\partial x_1} + \frac{\Delta x_1^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_1^2} + ...\right] \\ &- A_N\left[U_{kP}^m + \Delta x_2\frac{\partial U_{kP}^m}{\partial x_2} + \frac{\Delta x_2^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_2^2} + ...\right] \\ &- A_S\left[U_{kP}^m - \Delta x_3\frac{\partial U_{kP}^m}{\partial x_3} + \frac{\Delta x_3^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_3^2} + ...\right] \\ &- A_T\left[U_{kP}^m + \Delta x_3\frac{\partial U_{kP}^m}{\partial x_3} + \frac{\Delta x_3^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_3^2} + ...\right] \\ &- A_B\left[U_{kP}^m - \Delta x_2\frac{\partial U_{kP}^m}{\partial x_2} + \frac{\Delta x_2^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_2^2} + ...\right] - \left(\sum_{d=1}^{k-1} c_d U_{kP}^m + \sum_{d=k+1}^{n} c_d U_{kP}^m\right)\frac{\Delta t}{R_k}.\end{aligned}$$

We now rearrange terms to obtain

$$\begin{aligned}\Delta t T_{P,m} &= \Delta t\frac{\partial U_{kP}^m}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 U_{kP}^m}{\partial t^2} - (A_P + A_E + A_W + A_N + A_S + A_T + A_B - 1)U_{kP}^m \\ &+ (A_W - A_E)\Delta x_1\frac{\partial U_{kP}^m}{\partial x_1} + (A_S - A_N)\Delta x_2\frac{\partial U_{kP}^m}{\partial x_2} + (A_B - A_T)\Delta x_3\frac{\partial U_{kP}^m}{\partial x_3} \\ &- (A_W + A_E)\frac{\Delta x_1^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_1^2} - (A_S + A_N)\frac{\Delta x_2^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_2^2} - (A_B + A_T)\frac{\Delta x_3^2}{2}\frac{\partial^2 U_{kP}^m}{\partial x_3^2} \\ &- \left(\sum_{d=1}^{k-1} c_d U_{kP}^m + \sum_{d=k+1}^{n} c_d U_k\right)\frac{\Delta t}{R_k} + ...\end{aligned}$$

A general function $\psi(r)$ is considered for truncation error. Hence, we get

$$T_{P,m} = \frac{\partial U_{kP}^m}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 U_{kP}^m}{\partial t^2} + \frac{1}{R_k}\left[R_k K_k U_{kP}^m + v_1\frac{\partial U_{kP}^m}{\partial x_1} + v_2\frac{\partial U_{kP}^m}{\partial x_2} + v_3\frac{\partial U_k}{\partial x_3} - D_1\frac{\partial^2 U_k}{\partial x_1^2}\right.$$
$$\left. - D_2\frac{\partial^2 U_{kP}^m}{\partial x_2^2} - D_3\frac{\partial^2 U_{kP}^m}{\partial x_3^2} - \sum_{d=1}^{k-1} R_d Y_{k/d} K_d U_{kP}^m - \sum_{d=k+1}^{n} R_d Y_{k/d} K_d U_{kP}^m\right]$$
$$+ \frac{1}{R_k}\left[[1-\psi(r)]\frac{v_1\Delta x_1}{2}\frac{\partial^2 U_{kP}}{\partial x_1^2} + [1-\psi(r)]\frac{v_2\Delta x_2}{2}\frac{\partial^2 U_{kP}}{\partial x_2^2} + [1-\psi(r)]\frac{v_3\Delta x_3}{2}\frac{\partial^2 U_{kP}}{\partial x_3^2}\right]$$
$$+ O(\Delta x_1 + \Delta x_2 + \Delta x_3). \tag{12}$$

The flux limiter $\psi(r)$ is associated with the numerical diffusion terms in (12). Numerical diffusion is controlled when $|1-\psi(r)| \leq 1$ (that is, $0 \leq \psi(r) \leq 2$). This is a necessary condition for a scheme to be TVD.

5 Numerical Simulation for Three-Dimensional Test Problems

5.1 Three-Dimensional Multi-Directional Sequential Reactions

Sequential reaction with transport velocity in all three dimensions is considered in this problem. The three-dimensional transport of multi species involved in sequential reaction with solid and liquid phase degradation is governed by the following system of PDE's:

$$R_1\frac{\partial U_1}{\partial t} + v_1\frac{\partial U_1}{\partial x_1} + v_2\frac{\partial U_1}{\partial x_2} + v_3\frac{\partial U_1}{\partial x_3} - D_1\frac{\partial^2 U_1}{\partial x_1^2} - D_2\frac{\partial^2 U_1}{\partial x_2^2} - D_3\frac{\partial^2 U_1}{\partial x_3^2} = -K_1 R_1 U_1$$
$$R_2\frac{\partial U_2}{\partial t} + v_1\frac{\partial U_1}{\partial x_1} + v_2\frac{\partial U_1}{\partial x_2} + v_3\frac{\partial U_1}{\partial x_3} - D_1\frac{\partial^2 U_2}{\partial x_1^2} - D_2\frac{\partial^2 U_2}{\partial x_2^2} - D_3\frac{\partial^2 U_2}{\partial x_3^2} = K_1 R_1 U_1 - K_2 R_2 U_2$$
$$R_3\frac{\partial U_3}{\partial t} + v_1\frac{\partial U_1}{\partial x_1} + v_2\frac{\partial U_1}{\partial x_2} + v_3\frac{\partial U_1}{\partial x_3} - D_1\frac{\partial^2 U_3}{\partial x_1^2} - D_2\frac{\partial^2 U_3}{\partial x_2^2} - D_3\frac{\partial^2 U_3}{\partial x_3^2} = K_2 R_2 U_2 - K_3 R_3 U_3$$
$$R_4\frac{\partial U_4}{\partial t} + v_1\frac{\partial U_1}{\partial x_1} + v_2\frac{\partial U_1}{\partial x_2} + v_3\frac{\partial U_1}{\partial x_3} - D_1\frac{\partial^2 U_4}{\partial x_1^2} - D_2\frac{\partial^2 U_4}{\partial x_2^2} - D_3\frac{\partial^2 U_4}{\partial x_3^2} = K_3 R_3 U_3 - K_4 R_4 U_4$$

with the boundary conditions

$$U_k(0,0,0,t) = U_{k0}$$
$$\lim_{x_1\to\infty} U_k(x_1,x_2,x_3,t) = 0$$
$$\lim_{x_2\to\infty} U_k(x_1,x_2,x_3,t) = 0$$
$$\lim_{x_3\to\infty} U_k(x_1,x_2,x_3,t) = 0 \; k = 1,2,3,4.$$

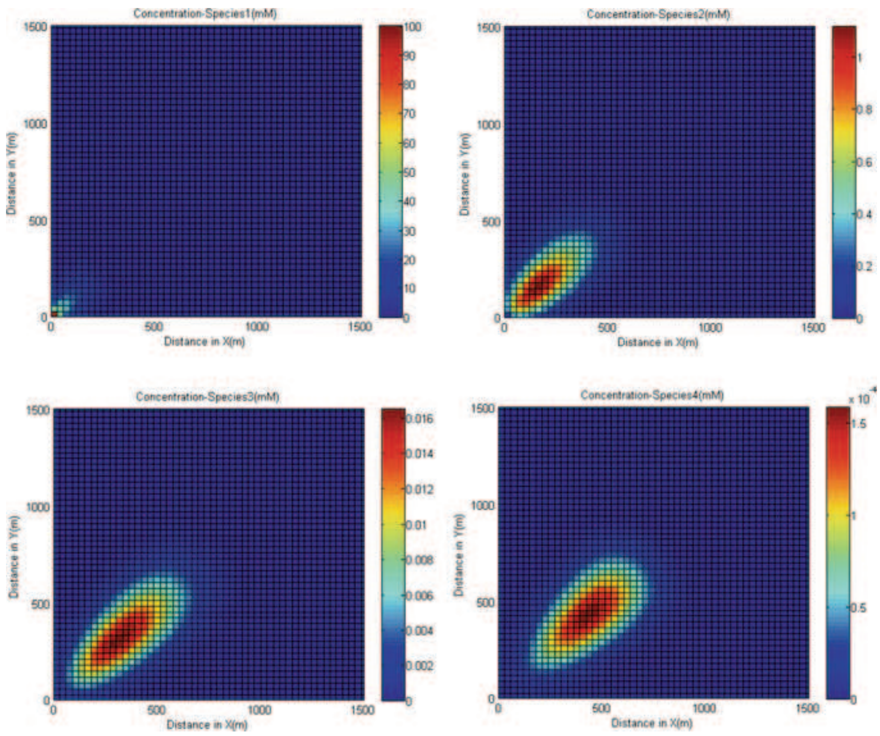

Fig. 2 Simulation for central difference limiter for 1000 days with sequential reaction

A constant amount of 100 mM for species-1 and zero mM for other three species at all times are injected at the origin. The concentration profile of four species transport for 1000 days is simulated numerically. Numerical simulation of this with central difference, van Leer limiter and Sweby limiter is shown in Fig. 2, Fig. 3, and Fig. 4, respectively. The parameters in Table 2 are used for numerical simulation.

5.2 Three Dimensional Multi-directional Serial–Parallel Reactions

Three-dimensional transport of multi-species with serial–parallel reversible reaction in both solid and liquid phase degradation is governed by the following system of PDEs:

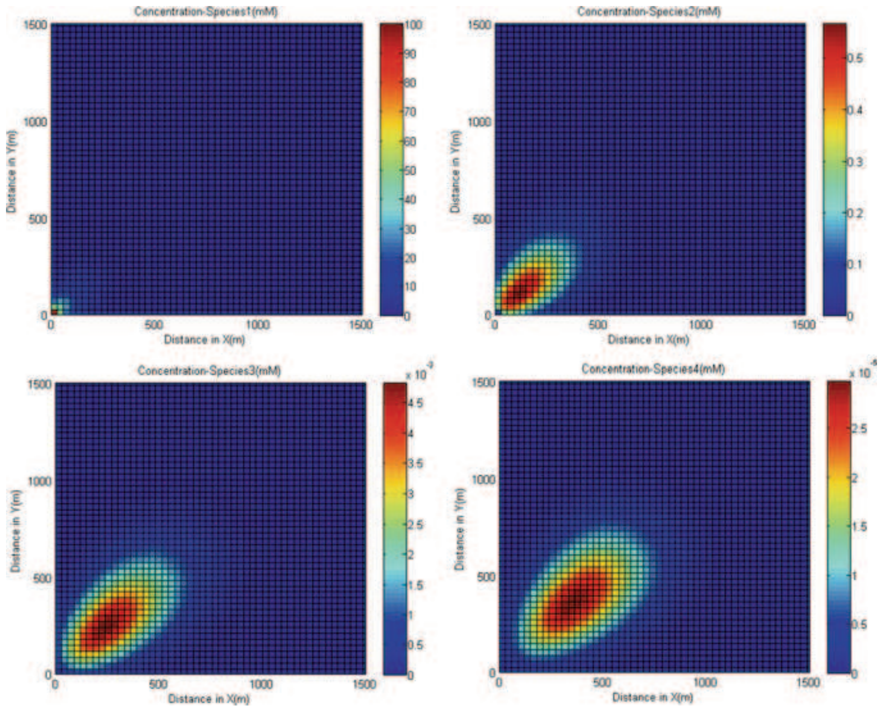

Fig. 3 Simulation for van Leer limiter for 1000 days with sequential reaction

$$
\begin{aligned}
R_1\frac{\partial U_1}{\partial t}+v_1\frac{\partial U_1}{\partial x_1}+v_2\frac{\partial U_1}{\partial x_2}+v_3\frac{\partial U_1}{\partial x_3}-D_1\frac{\partial^2 U_1}{\partial x_1^2}-D_2\frac{\partial^2 U_1}{\partial x_2^2}-D_3\frac{\partial^2 U_1}{\partial x_3^2} &= -K_1R_1U_1\\
R_2\frac{\partial U_2}{\partial t}+v_1\frac{\partial U_1}{\partial x_1}+v_2\frac{\partial U_1}{\partial x_2}+v_3\frac{\partial U_1}{\partial x_3}-D_1\frac{\partial^2 U_2}{\partial x_1^2}-D_2\frac{\partial^2 U_2}{\partial x_2^2}-D_3\frac{\partial^2 U_2}{\partial x_3^2} &= F_{2/1}Y_{2/1}K_1R_1U_1\\
&\quad -K_2R_2U_2\\
R_3\frac{\partial U_3}{\partial t}+v_1\frac{\partial U_1}{\partial x_1}+v_2\frac{\partial U_1}{\partial x_2}+v_3\frac{\partial U_1}{\partial x_3}-D_1\frac{\partial^2 U_3}{\partial x_1^2}-D_2\frac{\partial^2 U_3}{\partial x_2^2}-D_3\frac{\partial^2 U_3}{\partial x_3^2} &= F_{3/1}Y_{3/1}K_1R_1U_1\\
&\quad +F_{3/2}Y_{3/2}K_2R_2U_2\\
&\quad -K_3R_3U_3\\
R_4\frac{\partial U_4}{\partial t}+v_1\frac{\partial U_1}{\partial x_1}+v_2\frac{\partial U_1}{\partial x_2}+v_3\frac{\partial U_1}{\partial x_3}-D_1\frac{\partial^2 U_4}{\partial x_1^2}-D_2\frac{\partial^2 U_4}{\partial x_2^2}-D_3\frac{\partial^2 U_4}{\partial x_3^2} &= F_{4/2}Y_{4/2}K_2R_2U_2\\
&\quad +F_{4/3}Y_{4/3}K_3R_3U_3\\
&\quad -K_4R_4U_4
\end{aligned}
$$

with the boundary conditions

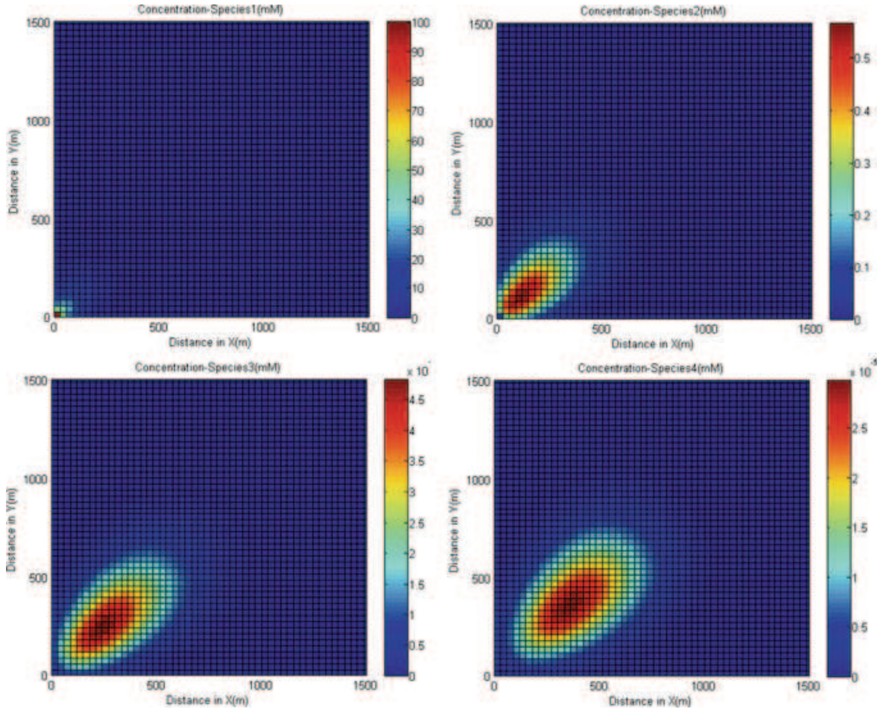

Fig. 4 Simulation for Sweby limiter for 1000 days with sequential reaction

Table 2 Parameters used for numerical simulation

Parameter	Value	Parameter	Value
U_{10}	100 mM (Constant source)	R_4	1.3
U_{10}	100 mM (Instantaneous/Point source)	K_1	$0.0007\,d^{-1}$
U_{20}	0	K_2	$0.0005\,d^{-1}$
U_{30}	0	K_3	$0.00045\,d^{-1}$
U_{40}	0	K_4	$0.00038\,d^{-1}$
D_1	$10\,m^2\,d^{-1}$	$F_{2/1}$	0.75
D_2	$10\,m^2\,d^{-1}$	$F_{3/1}$	0.25
D_3	$0.1\,m^2\,d^{-1}$	$F_{3/2}$	0.5
v_1	$1\,m\,d^{-1}$	$F_{4/2}$	0.5
v_2	$1\,m\,d^{-1}$	$F_{2/3}$	0.9
v_3	$0.1\,m\,d^{-1}$	$F_{4/3}$	0.1
R_1	5.3	$Y_{k/d}$	1 for all of them
R_2	1.9	T	1000 d
R_3	1.2	Δt	10
		Δx	30

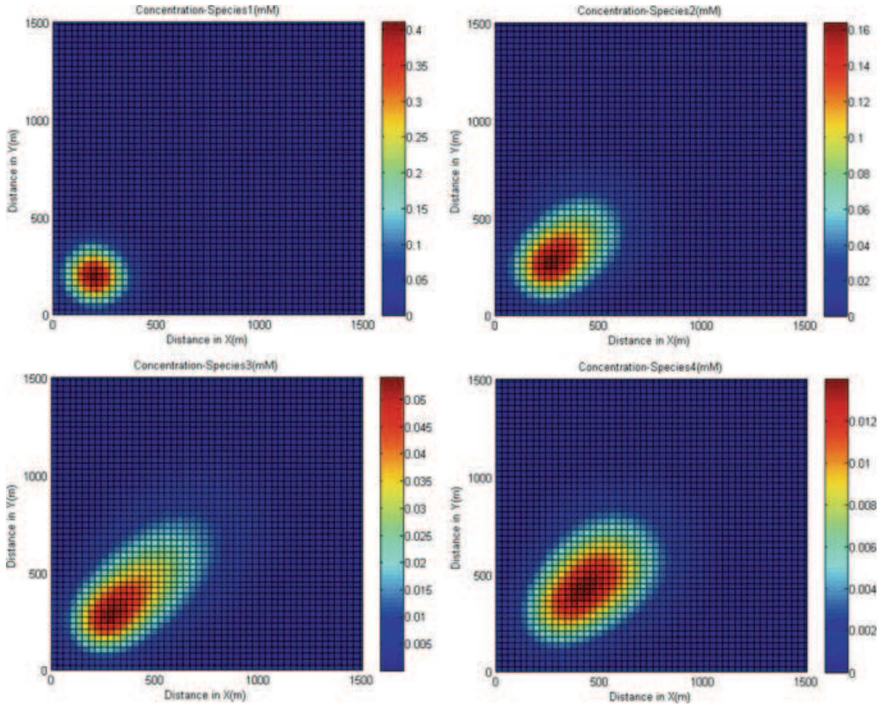

Fig. 5 Instantaneous or point injection simulation for van Albada limiter for 1000 days serial–parallel reversible reaction

$$
\begin{aligned}
U_k(0,0,0,0) &= U_{k0} \\
\lim_{x_1\to\infty} U_k(x_1,x_2,x_3,t) &= 0 \\
\lim_{x_2\to\infty} U_k(x_1,x_2,x_3,t) &= 0 \\
\lim_{x_3\to\infty} U_k(x_1,x_2,x_3,t) &= 0 \; k = 1,2,3,4.
\end{aligned}
$$

Instantaneous injection or point injection at time $t = 0$ is studied in this problem. An amount for 100 mM of species-1 and zero mM for other three species is injected at origin at time $t = 0$ and the movement of species is predicted for 1000 days. Numerical simulation of this with van Albada limiter, and Superbee limiter is shown in Fig. 5 and Fig. 6, respectively. The parameters in Table 2 are used for numerical simulation.

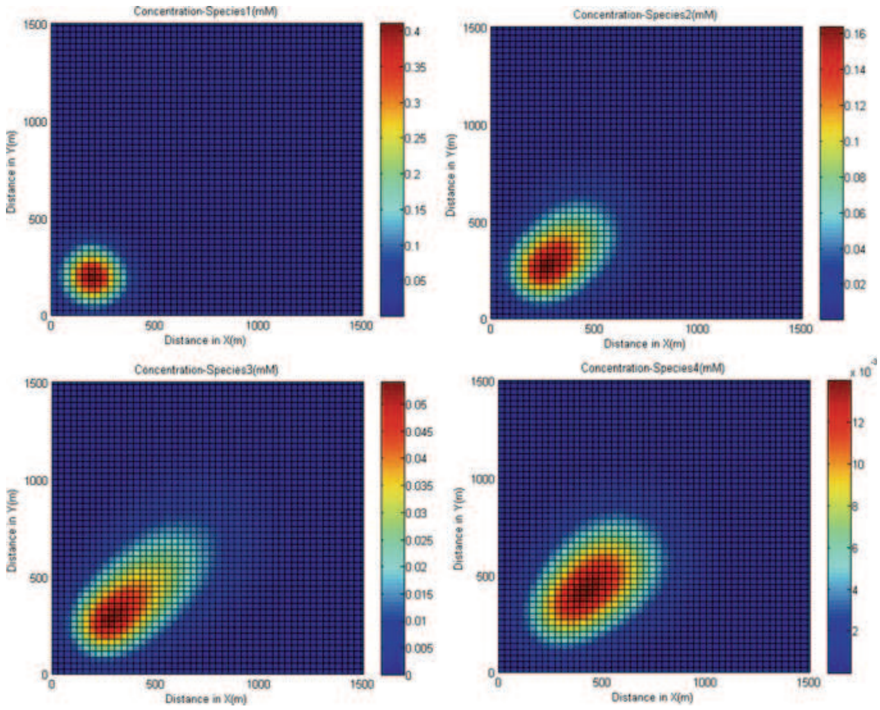

Fig. 6 Instantaneous or point injection simulation for Superbee limiter for 1000 days with serial–parallel reversible reaction

6 Summary and Conclusion

Multi-species transport equation in three dimensions with the first-order reaction network is considered in this article. Total variation diminishing finite volume scheme is applied for this problem. The stability and consistency conditions are derived. The necessary condition for flux limiter for controlling numerical diffusion is also derived. Numerical simulations are carried out for sequential reaction, reversible serial–parallel reaction problems with constant source and instantaneous or point source. Numerical simulations for four species transport are illustrated through graphs.

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