

Error analysis of finite difference methods for two-dimensional advection–dispersion–reaction equation

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Abstract

In this paper, the numerical errors associated with the finite difference solutions of two-dimensional advection–dispersion equation with linear sorption are obtained from a Taylor analysis and are removed from numerical solution. The error expressions are based on a general form of the corresponding difference equation. The variation of these numerical truncation errors is presented as a function of Peclet and Courant numbers in X and Y direction, a Sink/Source dimensionless number and new form of Peclet and Courant numbers in X – Y plane. It is shown that the Crank–Nicolson method is the most accurate scheme based on the truncation error analysis. The effects of these truncation errors on the numerical solution of a two-dimensional advection–dispersion equation with a first-order reaction or degradation are demonstrated by comparison with an analytical solution for predicting contaminant plume distribution in uniform flow field. Considering computational efficiency, an alternating direction implicit method is used for the numerical solution of governing equation. The results show that removing these errors improves numerical result and reduces differences between numerical and analytical solution.

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1. Introduction

Groundwater quality varies due to the chemical, geochemical, and biochemical reactions of the pollutants in the subsurface flow systems. To reliably predict the fate of contaminant transport in groundwater, an accurate numerical modeling is required.

There are many numerical investigations of advection–dispersion equation (transport equation). However, a few studies have been devoted to the more general advection–dispersion–reaction equation (ADRE). The numerical solution of ADRE has its complexity because of the reaction term. The reaction term accounts for degradation or adsorption, this term can cause numerical instability

problems. Ongoing research effort in this area reflects difficulty in solving the ADE by numerical methods for the cases such as advection-dominated problems, where the hyperbolic behavior of this equation is problematic especially in multi-dimensional ADE [1,2]. Also the solution of the transport equation (for advection-dominated problems), by many standard numerical procedures is plagued to some degree by two types of numerical problems. The first type is numerical dispersion due to the discretization of the governing equation. The second type of numerical problem is artificial oscillation [3].

Several approaches have been developed to improve the numerical accuracy. Among the numerical methods for solving ADRE, finite difference method (FDM) seems to be more popular for the ease of implementation and their relative simplicity [4–7]. However, finite element method (FEM) can easier handle complex geometries. There have been extensive debates as to

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Nomenclature

C	solute concentrations [ML^{-3}]	k_{num}	numerical first-order reaction rate coefficient [T^{-1}]
C_0	solute concentration in injected fluid [ML^{-3}]	Pe_{xx}	principal-term of Peclet number [–]
Cr_{xx}	principal-term of Courant number [–]	Pe_{xy}	cross-term of Peclet number [–]
Cr_{yy}	principal-term of Courant number [–]	Pe_{yy}	principal-term of Peclet number [–]
Cr_{xy}	cross-term of Courant number [–]	Sr	Sink/Source number [–]
D_{xx}	principal-term of dispersion coefficient [L^2T^{-1}]	t	time [T]
D_{yy}	principal-term of dispersion coefficient [L^2T^{-1}]	v	uniform flow velocity [LT^{-1}]
D_{xy}	cross-term of dispersion coefficient [L^2T^{-1}]	v_x	velocity component in X direction [LT^{-1}]
$D_{\text{num}xx}$	principal-term of numerical dispersion coefficient [L^2T^{-1}]	v_y	velocity component in Y direction [LT^{-1}]
$D_{\text{num}yy}$	principal-term of numerical dispersion coefficient [L^2T^{-1}]	$v_{\text{num}x}$	numerical velocity component in X direction [LT^{-1}]
$D_{\text{num}xy}$	cross-term of numerical dispersion coefficient [L^2T^{-1}]	$v_{\text{num}y}$	numerical velocity component in Y direction [LT^{-1}]
erfc	complementary error function [–]	Δx	length increment in X direction [L]
exp	exponential [–]	Δy	length increment in Y direction [L]
k	first-order reaction rate coefficient [T^{-1}]	Δt	time increment [T]
		\sum	summation [–]
		α_i	spatial weighting parameter in i direction [–]

whether FEM or FDM is preferable in groundwater modeling [11]. Some investigations showed that FDM introduces larger numerical errors than FEM [1,8–10].

Mixed Eulerian–Lagrangian methods are among the approaches that are used for eliminating numerical dispersion. MT3D code applies a mixed Eulerian–Lagrangian approach to solve the ADRE. This approach combines the strength of the method of characteristic to eliminate the numerical dispersion and the computational efficiency of the modified method of characteristics [3,12].

High-order finite difference methods are techniques that are used for a better accuracy and to eliminate the numerical dispersion [13–15]. Total-variation-diminishing (TVD) methods can be placed in this category. A large number of TVD schemes for solving advective transport equation can be found in the literature [11]. In spite of the promising performance of the high-order numerical methods, these schemes have their difficulties for programming and code implementing.

Although there are many studies that have applied FDM for two-dimensional ADE [7,11,16–18], the authors are not aware of any work on the truncation errors analysis of the FDM for the two-dimensional ADRE, except the recent work of the authors about explicit FDM [19].

Approximating differential equations in finite difference models by discretization introduces numerical errors (truncation error). In the case of transport equations like the advection–dispersion equation, numerical dispersion is a well-known consequence of truncation error [3,11,20,21]. Lantz [20] and Chaudhari [21] quantified numerical dispersion as a second-order error through examina-

tion of the truncated Taylor series approximation of an explicit FD solution of one-dimensional ADE. The effect of numerical dispersion has been considered in numerical studies by many researchers [1,22–27]. Notodarmojo et al. [24] presented a numerical model for phosphorus transport in soils and ground water with two-consecutive reactions. The model uses an explicit FD scheme and takes into account the influence of numerical dispersion although the effects of zero- and first-order truncation errors are neglected. Noye et al. discussed on the modified equivalent partial differential equation (MEPDE) truncation errors and estimated the accuracy of FDMs based on artificial damping and phase shifting property. They also compared amplitude response and relative wave speed obtained in a series form using the coefficients of MEPDE to examine the accuracy of different FDMs [26,27].

The numerical dispersion is the only truncation error for the case of advection–dispersion equation. However for the more general transport equation (e.g., with reaction) other truncation errors are also introduced [4,19,28,29].

The primary objectives of this paper are to analysis the errors of the general form of FDM for two-dimensional ADRE. Errors are expressed in the form of dimensionless numbers. These truncation errors are compared for different schemes with respect to dimensionless numbers. In the end, it has been shown that removing these numerical errors improves the results of FD solution of ADRE and leads to a more accurate numerical solution. Consideration computational efficiency, an alternating direction implicit (ADI) method is used. ADI method has a second-order accuracy and

is unconditionally stable. Therefore this technique is commonly used to solve two-dimensional ADE [7].

2. Finite difference approximation of ADRE

The two-dimensional advection–dispersion equation with a first-order reaction or degradation is written as [3,11]:

$$\frac{\partial C}{\partial t} = D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{xy} \frac{\partial^2 C}{\partial x \partial y} + D_{yx} \frac{\partial^2 C}{\partial y \partial x} + D_{yy} \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} - kC, \quad (1a)$$

where C is dissolved concentration [ML^{-3}], t is time [T], k is first-order reaction rate coefficient [T^{-1}], D_{xx} , D_{yy} are principal-terms of dispersion coefficient [L^2T^{-1}], D_{xy} , D_{yx} are cross-terms of dispersion coefficient [L^2T^{-1}], and v_x , v_y are velocity component in X and Y directions [LT^{-1}]. The equation is for the cases of negligible spatial variability of the dispersion coefficient and velocity components and in these cases D_{xy} and D_{yx} are equal, so simplified form of Eq. (1a) is presented [3,11]:

$$\frac{\partial C}{\partial t} = D_{xx} \frac{\partial^2 C}{\partial x^2} + 2D_{xy} \frac{\partial^2 C}{\partial x \partial y} + D_{yy} \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} - kC. \quad (1b)$$

The general form of FD approximation of Eq. (1), using ω as the temporal weighting factor and α_1 and α_2 as the spatial weighting parameters in X and Y directions, leading to the following FD equation [4]:

$$\begin{aligned} \frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t} = & D_{xx} \left[(1-\omega) \frac{C_{i+1,j}^n - 2C_{i,j}^n + C_{i-1,j}^n}{\Delta x^2} \right. \\ & \left. + \omega \frac{C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}}{\Delta x^2} \right] \\ & + D_{yy} \left[(1-\omega) \frac{C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n}{\Delta y^2} \right. \\ & \left. + \omega \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{\Delta y^2} \right] \\ & + D_{xy} \left[(1-\omega) \frac{C_{i+1,j+1}^n - C_{i+1,j-1}^n - C_{i-1,j+1}^n + C_{i-1,j-1}^n}{2\Delta x \Delta y} \right. \\ & \left. + \omega \frac{C_{i+1,j+1}^{n+1} - C_{i+1,j-1}^{n+1} - C_{i-1,j+1}^{n+1} + C_{i-1,j-1}^{n+1}}{2\Delta x \Delta y} \right] \\ & - v_x \left[(1-\omega) \frac{(1-\alpha_1)C_{i,j}^n + \alpha_1 C_{i+1,j}^n - (1-\alpha_1)C_{i-1,j}^n - \alpha_1 C_{i,j}^n}{\Delta x} \right. \\ & \left. + \omega \frac{(1-\alpha_1)C_{i,j}^{n+1} + \alpha_1 C_{i+1,j}^{n+1} - (1-\alpha_1)C_{i-1,j}^{n+1} - \alpha_1 C_{i,j}^{n+1}}{\Delta x} \right] \\ & - v_y \left[(1-\omega) \frac{(1-\alpha_2)C_{i,j}^n + \alpha_2 C_{i,j+1}^n - (1-\alpha_2)C_{i,j-1}^n - \alpha_2 C_{i,j}^n}{\Delta y} \right. \\ & \left. + \omega \frac{(1-\alpha_2)C_{i,j}^{n+1} + \alpha_2 C_{i,j+1}^{n+1} - (1-\alpha_2)C_{i,j-1}^{n+1} - \alpha_2 C_{i,j}^{n+1}}{\Delta y} \right] \\ & - k \left[(1-\omega)C_{i,j}^n + \omega C_{i,j}^{n+1} \right], \quad (2) \end{aligned}$$

where Δt is the time increment [T], and Δx and Δy are the length increment [L] in X and Y directions. The superscript n refers to time step level and the subscripts i and j refer to the nodal number in X and Y directions.

The general form of Eq. (2) reduces to the explicit form when the temporal weighting factor ω is 0.0 and it reduces to the fully implicit form when $\omega = 1.0$. For $\omega = 0.5$, the numerical method is referred to as the central-in-time or the Crank–Nicolson scheme.

The value of α_1 and α_2 determine the type of spatial discretization, and the most obvious choice of α_1 and α_2 is 0.5, which is referred to as the central in space scheme. An alternative spatial weighting scheme is the upstream or upwind scheme with positive velocity ($v_x, v_y > 0$) when $\alpha_1 = \alpha_2 = 0.0$ or with negative velocity ($v_x, v_y < 0$) when $\alpha_1 = \alpha_2 = 1.0$.

A Taylor series expansion of C about point (i,j) is used to determine the form of the truncation errors in two-dimensional ADRE [4,19,29]. If the same approach is used and the third- and higher-order spatial derivatives are neglected, as they are not present in the original equation, then

$$C_{i\pm 1,j}^n = C_{i,j}^n \pm \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C}{\partial x^2} + O(\Delta x^3), \quad (3)$$

$$C_{i,j\pm 1}^n = C_{i,j}^n \pm \Delta y \frac{\partial C}{\partial y} + \frac{\Delta y^2}{2} \frac{\partial^2 C}{\partial y^2} + O(\Delta y^3), \quad (4)$$

$$\begin{aligned} C_{i\pm 1,j-1}^n &= C_{i\pm 1,j}^n - \Delta y \frac{\partial C}{\partial y} \Big|_{i\pm 1,j} + \frac{\Delta y^2}{2} \frac{\partial^2 C}{\partial y^2} \Big|_{i\pm 1,j} + O(\Delta y^3) \\ &= C_{i,j}^n \pm \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C}{\partial x^2} - \Delta y \frac{\partial C}{\partial y} \\ &\quad - \frac{(\pm \Delta x) \times (\Delta y)}{2} \frac{\partial^2 C}{\partial x \partial y} + \frac{\Delta y^2}{2} \frac{\partial^2 C}{\partial y^2} + O(\Delta x^3) \\ &\quad + O(\Delta y^3) + O(\Delta x^2 \Delta y) + O(\Delta x \Delta y^2), \quad (5a) \end{aligned}$$

$$\begin{aligned} C_{i\pm 1,j+1}^n &= C_{i\pm 1,j}^n + \Delta y \frac{\partial C}{\partial y} \Big|_{i\pm 1,j} + \frac{\Delta y^2}{2} \frac{\partial^2 C}{\partial y^2} \Big|_{i\pm 1,j} + O(\Delta y^3) \\ &= C_{i,j}^n \pm \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C}{\partial x^2} + \Delta y \frac{\partial C}{\partial y} \\ &\quad + \frac{(\pm \Delta x) \times (\Delta y)}{2} \frac{\partial^2 C}{\partial x \partial y} + \frac{\Delta y^2}{2} \frac{\partial^2 C}{\partial y^2} + O(\Delta x^3) \\ &\quad + O(\Delta y^3) + O(\Delta x^2 \Delta y) + O(\Delta x \Delta y^2). \quad (5b) \end{aligned}$$

If Taylor series expansion of C at time step $n + \frac{1}{p}$ about n time step is also used then

$$C_{i,j}^{n+\frac{1}{p}} = C_{i,j}^n + \sum_{m=1}^{\infty} \frac{(\Delta t/p)^m}{m!} \frac{\partial^m C}{\partial t^m}, \quad (6)$$

where p is the interim step between two sequential steps.

The second- and higher-order temporal derivatives of C are written in terms of spatial derivatives of C using the differentiated form of Eq. (1), and again the

third- and higher-order spatial derivatives (in X or Y directions) are neglected [4,19,29]. Then in general for $m \geq 2$:

$$\begin{aligned} \frac{\partial^m C}{\partial t^m} \approx & (-1)^m \left[-mk^{m-1}D_{xx} + \frac{m(m-1)}{2}k^{m-2}v_x^2 \right] \frac{\partial^2 C}{\partial x^2} \\ & + (-1)^m \left[-mk^{m-1}D_{yy} + \frac{m(m-1)}{2}k^{m-2}v_y^2 \right] \frac{\partial^2 C}{\partial y^2} \\ & + (-1)^m [-2mk^{m-1}D_{xy} + m(m-1)k^{m-2}v_x v_y] \frac{\partial^2 C}{\partial x \partial y} \\ & + (-1)^m [mk^{m-1}v_x] \frac{\partial C}{\partial x} + (-1)^m [mk^{m-1}v_y] \frac{\partial C}{\partial y} \\ & + (-1)^m k^m C. \end{aligned} \tag{7}$$

Therefore Eq. (6) is written as

$$\begin{aligned} C_{i,j}^{n+\frac{1}{p}} \approx & C_{i,j}^n + \frac{\Delta t}{p} \frac{\partial C}{\partial t} + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m \\ & \times \left\{ \left[-mk^{m-1}D_{xx} + \frac{m(m-1)}{2}k^{m-2}v_x^2 \right] \frac{\partial^2 C}{\partial x^2} \right. \\ & + \left[-mk^{m-1}D_{yy} + \frac{m(m-1)}{2}k^{m-2}v_y^2 \right] \frac{\partial^2 C}{\partial y^2} \\ & + [-2mk^{m-1}D_{xy} + m(m-1)k^{m-2}v_x v_y] \frac{\partial^2 C}{\partial x \partial y} \\ & \left. + [mk^{m-1}v_x] \frac{\partial C}{\partial x} + [mk^{m-1}v_y] \frac{\partial C}{\partial y} + k^m C \right\}. \end{aligned} \tag{8}$$

It is noticed that the transport parameters are assumed constant only within each combination of time and depth increments in finite difference calculation. Inserting Eq. (8) in Eqs. (3)–(5) for time level $n + \frac{1}{p}$ and neglecting the spatial derivatives of third- and higher-order, for time level $n + \frac{1}{p}$ we have,

$$\begin{aligned} C_{i\pm 1,j}^{n+\frac{1}{p}} = & C_{i,j}^n + \frac{\Delta t}{p} \frac{\partial C}{\partial t} + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{(m-1)!} (-1)^m \\ & \times \left\{ \left[-k^{m-1}D_{xx} + \frac{(m-1)}{2}k^{m-2}v_x^2 \right] \frac{\partial^2 C}{\partial x^2} \right. \\ & + \left[-k^{m-1}D_{yy} + \frac{(m-1)}{2}k^{m-2}v_y^2 \right] \frac{\partial^2 C}{\partial y^2} \\ & + [-2k^{m-1}D_{xy} + (m-1)k^{m-2}v_x v_y] \frac{\partial^2 C}{\partial x \partial y} \\ & + [mk^{m-1}v_x] \frac{\partial C}{\partial x} + [k^{m-1}v_y] \frac{\partial C}{\partial y} + \frac{k^m}{m} C \left. \right\} \\ & \pm \Delta x \left\{ \frac{\partial C}{\partial x} + \frac{\Delta t}{p} \left[-v_x \frac{\partial^2 C}{\partial x^2} - v_y \frac{\partial^2 C}{\partial x \partial y} - k \frac{\partial C}{\partial x} \right] \right. \\ & + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{(m-1)!} (-1)^m \left\{ [k^{m-1}v_x] \frac{\partial^2 C}{\partial x^2} + [k^{m-1}v_y] \frac{\partial^2 C}{\partial x \partial y} \right. \\ & + (-1)^m \frac{k^m}{m} \frac{\partial C}{\partial x} \left. \right\} + \frac{\Delta x^2}{2} \left\{ \frac{\partial^2 C}{\partial x^2} + \frac{\Delta t}{p} \left[-k \frac{\partial^2 C}{\partial x^2} \right] \right. \\ & \left. + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m k^m \frac{\partial^2 C}{\partial x^2} \right\} \end{aligned} \tag{9}$$

and

$$\begin{aligned} C_{i,j\pm 1}^{n+\frac{1}{p}} = & C_{i,j}^n + \frac{\Delta t}{p} \frac{\partial C}{\partial t} + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m \\ & \times \left\{ \left[-k^{m-1}D_{xx} + \frac{(m-1)}{2}k^{m-2}v_x^2 \right] \frac{\partial^2 C}{\partial x^2} \right. \\ & + \left[-k^{m-1}D_{yy} + \frac{(m-1)}{2}k^{m-2}v_y^2 \right] \frac{\partial^2 C}{\partial y^2} \\ & + [-2k^{m-1}D_{xy} + (m-1)k^{m-2}v_x v_y] \frac{\partial^2 C}{\partial x \partial y} \\ & + [k^{m-1}v_x] \frac{\partial C}{\partial x} + [k^{m-1}v_y] \frac{\partial C}{\partial y} + \frac{k^m}{m} C \left. \right\} \\ & \pm \Delta y \left\{ \frac{\partial C}{\partial y} + \frac{\Delta t}{p} \left[-v_y \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial^2 C}{\partial y \partial x} - k \frac{\partial C}{\partial y} \right] \right. \\ & + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m (-1)^m}{(m-1)!} \left\{ [k^{m-1}v_x] \frac{\partial^2 C}{\partial x \partial y} + [k^{m-1}v_y] \frac{\partial^2 C}{\partial y^2} \right. \\ & + \frac{k^m}{m} \frac{\partial C}{\partial y} \left. \right\} + \frac{\Delta y^2}{2} \left\{ \frac{\partial^2 C}{\partial y^2} + \frac{\Delta t}{2} \left[-k \frac{\partial^2 C}{\partial y^2} \right] \right. \\ & \left. + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m k^m \frac{\partial^2 C}{\partial y^2} \right\}. \end{aligned} \tag{10}$$

Also we have,

$$\begin{aligned} C_{i\pm 1,j\mp 1}^{n+\frac{1}{p}} = & C_{i,j}^n + \frac{\Delta t}{p} \frac{\partial C}{\partial t} + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m (-1)^m}{(m-1)!} \\ & \times \left\{ \left[-k^{m-1}D_{xx} + \frac{(m-1)}{2}k^{m-2}v_x^2 \right] \frac{\partial^2 C}{\partial x^2} \right. \\ & + \left[-k^{m-1}D_{yy} + \frac{(m-1)}{2}k^{m-2}v_y^2 \right] \frac{\partial^2 C}{\partial y^2} \\ & + [-2k^{m-1}D_{xy} + (m-1)k^{m-2}v_x v_y] \frac{\partial^2 C}{\partial x \partial y} \\ & + [k^{m-1}v_x] \frac{\partial C}{\partial x} + [k^{m-1}v_y] \frac{\partial C}{\partial y} + \frac{k^m}{m} C \left. \right\} \\ & \pm \Delta x \left\{ \frac{\partial C}{\partial x} + \frac{\Delta t}{p} \left[-v_x \frac{\partial^2 C}{\partial x^2} - v_y \frac{\partial^2 C}{\partial x \partial y} - k \frac{\partial C}{\partial x} \right] \right. \\ & + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m (-1)^m}{(m-1)!} \left\{ [k^{m-1}v_x] \frac{\partial^2 C}{\partial x^2} + [k^{m-1}v_y] \frac{\partial^2 C}{\partial x \partial y} \right. \\ & + \frac{k^m}{m} \frac{\partial C}{\partial x} \left. \right\} + \frac{\Delta x^2}{2} \left\{ \frac{\partial^2 C}{\partial x^2} + \frac{\Delta t}{p} \left[-k \frac{\partial^2 C}{\partial x^2} \right] \right. \\ & + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m k^m \frac{\partial^2 C}{\partial x^2} \left. \right\} \\ & \mp \Delta y \left\{ \frac{\partial C}{\partial y} + \frac{\Delta t}{p} \left[-v_y \frac{\partial^2 C}{\partial y^2} - v_x \frac{\partial^2 C}{\partial y \partial x} - k \frac{\partial C}{\partial y} \right] \right. \\ & + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m (-1)^m}{(m-1)!} \left\{ [k^{m-1}v_x] \frac{\partial^2 C}{\partial x \partial y} + [k^{m-1}v_y] \frac{\partial^2 C}{\partial y^2} \right. \\ & + \frac{k^m}{m} \frac{\partial C}{\partial y} \left. \right\} + \frac{\Delta y^2}{2} \left\{ \frac{\partial^2 C}{\partial y^2} + \frac{\Delta t}{p} \left[-k \frac{\partial^2 C}{\partial y^2} \right] \right. \\ & \left. + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m k^m \frac{\partial^2 C}{\partial y^2} \right\} \end{aligned}$$

$$\begin{aligned}
 & + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m k^m \frac{\partial^2 C}{\partial y^2} \left. \right\} + \frac{(\pm \Delta x) \times (\mp \Delta y)}{2} \\
 & \times \left\{ \frac{\partial^2 C}{\partial x \partial y} + \frac{\Delta t}{p} \left[-k \frac{\partial^2 C}{\partial x \partial y} \right] \right. \\
 & \left. + \sum_{m=2}^{\infty} \frac{(\Delta t/p)^m}{m!} (-1)^m k^m \frac{\partial^2 C}{\partial x \partial y} \right\}. \tag{11}
 \end{aligned}$$

3. Numerical solution

There are limitations for the explicit method based on the stability criterion associated with them, so the size of time steps cannot exceed a certain value. Due to these limitations, the explicit scheme is not commonly used. To overcome, the stability restrictions, in this work an implicit numerical method is considered. Applying a conventional implicit method causes the resulting system of linear algebraic equations to be pentadiagonal. Therefore for computational efficiency, an alternating direction implicit (ADI) method is used in order to have a tridiagonal system of linear algebraic equations. ADI scheme includes two stages of calculation for each time step.

The central-in-space weighting scheme for spatial discretization often leads to artificial oscillation (overshoot or undershoot) in the numerical solution. This is especially true when a sharp concentration front is present in advection-dominated cases [11]. The problem of artificial oscillation can be overcome through the use of upstream weighting. Upstream weighting tends to aggravate the numerical dispersion; therefore, upstream ADI method was selected for studying truncation errors. Then the simplified form of Eq. (2) at stage (1) of ADI scheme for the case of $\alpha_1 = \alpha_2 = 0.0$ can be written as follows:

$$\begin{aligned}
 \frac{C_{i,j}^{n+1/2} - C_{i,j}^n}{\Delta t/2} &= D_{xx} \left[\frac{C_{i+1,j}^{n+1/2} - 2C_{i,j}^{n+1/2} + C_{i-1,j}^{n+1/2}}{\Delta x^2} \right] \\
 &+ D_{yy} \left[\frac{C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n}{\Delta y^2} \right] \\
 &+ D_{xy} \left[\frac{C_{i+1,j+1}^{n+1/2} - C_{i+1,j-1}^{n+1/2} - C_{i-1,j+1}^{n+1/2} + C_{i-1,j-1}^{n+1/2}}{2\Delta x \Delta y} \right] \\
 &- v_x \left[\frac{C_{i,j}^{n+1/2} - C_{i-1,j}^{n+1/2}}{\Delta x} \right] - v_y \left[\frac{C_{i,j}^n - C_{i,j-1}^n}{\Delta y} \right] \\
 &- kC_{i,j}^{n+1/2}. \tag{12}
 \end{aligned}$$

Substituting Eqs. (3)–(5) for time level (n) and Eqs. (9)–(11) for time level (n + 1/2) in Eq. (12) and by simplifying the resulting equation for time step (n) gives:

$$\begin{aligned}
 \frac{\partial C}{\partial t} &= \left\{ D_{xx} - k\Delta t D_{xx} - \frac{v_x k \Delta t \Delta x}{4} + \frac{v_x \Delta x}{2} + \frac{v_x^2 \Delta t}{2} \right. \\
 &- \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m \left(1 + \frac{k\Delta t}{2} \right) \\
 &\times \left[-k^{m-1} D_{xx} + \frac{(m-1)}{2} k^{m-2} v_x^2 \right] \\
 &- \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m-1)!} (-1)^m k^{m-1} v_x^2 + \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m)!} (-1)^m k^m \\
 &\times \left(\frac{v_x \Delta x}{2} + D_{xx} \right) \left. \right\} \frac{\partial^2 C}{\partial x^2} + \left\{ D_{yy} - \frac{k\Delta t D_{yy}}{2} + \frac{v_y \Delta y}{2} \right. \\
 &- \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m \left(1 + \frac{k\Delta t}{2} \right) \left[-k^{m-1} D_{yy} \right. \\
 &\left. + \frac{(m-1)}{2} k^{m-2} v_y^2 \right] \left. \right\} \frac{\partial^2 C}{\partial y^2} + \left\{ 2D_{xy} - 2k\Delta t D_{xy} \right. \\
 &+ \frac{v_x v_y \Delta t}{2} - \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m \left(1 + \frac{k\Delta t}{2} \right) \left[-2k^{m-1} D_{xy} \right. \\
 &\left. + (m-1)k^{m-2} v_x v_y \right] - \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m)!} (-1)^m k^{m-1} \\
 &\times \left[-mv_x v_y + 2kD_{xy} \right] \left. \right\} \frac{\partial^2 C}{\partial x \partial y} - \left\{ v_x - k\Delta t v_x \right. \\
 &+ \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m k^{m-1} v_x \left(1 + \frac{k\Delta t}{2} \right) \\
 &+ \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m)!} (-1)^m k^m v_x \left. \right\} \frac{\partial C}{\partial x} \\
 &- \left\{ v_y - \frac{k\Delta t v_y}{2} + \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m k^{m-1} v_y \right. \\
 &\times \left(1 + \frac{k\Delta t}{2} \right) \left. \right\} \frac{\partial C}{\partial y} - \left\{ k - \frac{k^2 \Delta t}{2} + \sum_{m=2}^{\infty} \frac{\Delta t^{m-1}}{(m)!} (-1)^m k^m \right. \\
 &\times \left(1 + \frac{k\Delta t}{2} \right) \left. \right\} C. \tag{13}
 \end{aligned}$$

For stage (2) FD discretization leads to

$$\begin{aligned}
 \frac{C_{i,j}^{n+1} - C_{i,j}^{n+1/2}}{\Delta t/2} &= D_{xx} \left[\frac{C_{i+1,j}^{n+1/2} - 2C_{i,j}^{n+1/2} + C_{i-1,j}^{n+1/2}}{\Delta x^2} \right] \\
 &+ D_{yy} \left[\frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{\Delta y^2} \right] \\
 &+ D_{xy} \left[\frac{C_{i+1,j+1}^{n+1} - C_{i+1,j-1}^{n+1} - C_{i-1,j+1}^{n+1} + C_{i-1,j-1}^{n+1}}{2\Delta x \Delta y} \right] \\
 &- v_x \left[\frac{C_{i,j}^{n+1/2} - C_{i-1,j}^{n+1/2}}{\Delta x} \right] - v_y \left[\frac{C_{i,j}^{n+1} - C_{i,j-1}^{n+1}}{\Delta y} \right] - kC_{i,j}^{n+1}. \tag{14}
 \end{aligned}$$

Substituting Eqs. (3)–(5) for time level $(n + 1/2)$ and Eqs. (9)–(11) for time level $(n + 1)$ in Eq. (14) and simplifying the resulting equation for time step $(n + 1/2)$ gives

$$\begin{aligned} \frac{\partial C}{\partial t} = & \left\{ D_{xx} - \frac{k\Delta t}{2} D_{xx} + \frac{v_x \Delta x}{2} - \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m \right. \\ & \times \left(1 + \frac{k\Delta t}{2} \right) \left[-k^{m-1} D_{xx} + \frac{(m-1)}{2} k^{m-2} v_x^2 \right] \left. \right\} \frac{\partial^2 C}{\partial x^2} \\ & + \left\{ D_{yy} - k\Delta t D_{yy} - \frac{v_y k \Delta t \Delta y}{4} + \frac{v_y \Delta y}{2} + \frac{\Delta t v_y^2}{2} \right. \\ & - \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m \left(1 + \frac{k\Delta t}{2} \right) \left[-k^{m-1} D_{yy} \right. \\ & \left. \left. + \frac{(m-1)}{2} k^{m-2} v_y^2 \right] - \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m-1)!} (-1)^m k^{m-1} v_y^2 \right. \\ & \left. + \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m)!} (-1)^m k^m \left(\frac{k_y \Delta y}{2} + D_{yy} \right) \right\} \frac{\partial^2 C}{\partial y^2} \\ & + \left\{ 2D_{xy} - 2k\Delta t D_{xy} + \frac{v_x v_y \Delta t}{2} - \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m \right. \\ & \times \left(1 + \frac{k\Delta t}{2} \right) \left[-2k^{m-1} D_{xy} + (m-1) k^{m-2} v_x v_y \right] \\ & - \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m)!} (-1)^m k^{m-1} \left[-m v_x v_y + 2k D_{xy} \right] \left. \right\} \frac{\partial^2 C}{\partial x \partial y} \\ & - \left\{ v_x - \frac{k\Delta t}{2} v_x + \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m k^{m-1} v_x \left(1 + \frac{k\Delta t}{2} \right) \right\} \\ & \times \frac{\partial C}{\partial x} - \left\{ v_y - k\Delta t v_y + \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m-1)!} (-1)^m k^{m-1} v_y \right. \\ & \times \left(1 + \frac{k\Delta t}{2} \right) + \sum_{m=2}^{\infty} \frac{(\Delta t/2)^m}{(m)!} (-1)^m k^m v_y \left. \right\} \frac{\partial C}{\partial y} \\ & - \left\{ k - \frac{k^2 \Delta t}{2} + \sum_{m=2}^{\infty} \frac{(\Delta t/2)^{m-1}}{(m)!} (-1)^m k^m \left(1 + \frac{k\Delta t}{2} \right) \right\} C. \end{aligned} \quad (15)$$

4. Truncation error formulations in dimensionless form

A comparison between Eq. (13) for step (1) and Eq. (15) for stage (2) and the original governing differential equation shows that discretization introduces three forms of truncation error within each solution stage. They can be identified as a second-order truncation error or numerical dispersion in X and Y directions, D_{numxx} and D_{numyy} , and cross-term, D_{numxy} . If the two stages of ADI method is combined, Eqs. (12) and (14), numerical errors are also combined for both stages and we have only three terms for dispersion (D_{numxx} , D_{numyy} , D_{numxy}), two terms for numerical velocity

(v_{numx} , v_{numy}) and one term for numerical reaction coefficient. Truncation errors are obtained for this case. Therefore the numerical dispersions are as follows:

$$\begin{aligned} D_{numxx} = & -\frac{5k\Delta t D_{xx}}{4} - \frac{v_x k \Delta t \Delta x}{4} + \frac{v_x \Delta x}{2} + \frac{v_x^2 \Delta t}{2} \\ & - \sum_{m=2}^{\infty} \frac{(\Delta t)^{m-1}}{(m-1)!} (-1)^m k^{m-2} v_x^2 \left[-k D_{xx} + \frac{(m-1)}{2} v_x^2 \right] \\ & \times \left(1 + \frac{k\Delta t}{2} + \frac{k\Delta t}{2^{m+1}} \right) + \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{2^m (m)!} (-1)^m k^{m-1} \\ & \times \left[\frac{k v_x \Delta x}{2} + k D_{xx} - m v_x^2 \right], \end{aligned} \quad (16)$$

$$\begin{aligned} D_{numyy} = & -\frac{5k\Delta t D_{yy}}{4} - \frac{v_y k \Delta t \Delta y}{2} + \frac{v_y \Delta y}{2} + \frac{v_y^2 \Delta t}{2} \\ & - \sum_{m=2}^{\infty} \frac{(\Delta t)^{m-1}}{(m-1)!} (-1)^m k^{m-2} v_x^2 \left[-k D_{yy} + \frac{(m-1)}{2} v_y^2 \right] \\ & \times \left(1 + \frac{k\Delta t}{2} + \frac{k\Delta t}{2^{m+1}} \right) + \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{2^m (m)!} (-1)^m k^{m-1} \\ & \times \left[\frac{k v_y \Delta y}{2} + k D_{yy} - m v_y^2 \right], \end{aligned} \quad (17)$$

$$\begin{aligned} D_{numxy} = & -3k\Delta t D_{xy} + v_x v_y \Delta t \\ & - \sum_{m=2}^{\infty} \frac{(\Delta t)^{m-1}}{(m-1)!} (-1)^m k^{m-2} \left[-2k D_{xy} + (m-1) v_x v_y \right] \\ & \times \left(1 + \frac{k\Delta t}{2} + \frac{k\Delta t}{2^{m+1}} \right) + \frac{1}{2} \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{m!} (-1)^m k^{m-1} \\ & \times \left[2k D_{xy} - m v_x v_y \right] + \frac{1}{2} \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{2^{m-1} m!} (-1)^m k^{m-1} \\ & \times \left[k D_{xy} - m v_x v_y \right]. \end{aligned} \quad (18)$$

A first-order truncation error or numerical ground water velocity in X and Y directions, v_{numx} and v_{numy} can be written as follows for step (1):

$$\begin{aligned} V_{numx} = & -\frac{5k\Delta t v_x}{4} + \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{2^m m!} (-1)^m k^m v_x \left(1 + \frac{m}{2} \right) \\ & + \frac{1}{2} \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{(m-1)!} (-1)^m k^m v_x, \end{aligned} \quad (19)$$

$$\begin{aligned} V_{numy} = & -\frac{5k\Delta t v_y}{4} + \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{m!} (-1)^m k^m v_y \left(1 + \frac{m}{2} \right) \\ & + \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{2^{m+1} (m-1)!} (-1)^m k^m v_y. \end{aligned} \quad (20)$$

And a zero-order truncation error or numerical reaction coefficient,

$$K_{num} = -\frac{3k^2 \Delta t}{4} + \frac{1}{2} \sum_{m=2}^{\infty} \frac{(\Delta t)^m}{(m)!} (-1)^m k^{m+1} \left(1 + \frac{1}{2^m} \right). \quad (21)$$

Using the Peclet number, Pe , Courant number, Cr , in X and Y directions, Sink/Source number, Sr , and introducing cross-term of Peclet and Courant numbers as follows:

$$Cr_{xx} = \frac{v_x \Delta t}{\Delta x}, \tag{22a}$$

$$Cr_{yy} = \frac{v_y \Delta t}{\Delta y}, \tag{22b}$$

$$Cr_{xy} = \frac{(v_x v_y)^{0.5} \Delta t}{(\Delta x \Delta y)^{0.5}}, \tag{22c}$$

$$Pe_{xx} = \frac{v_x \Delta x}{D_{xx}}, \tag{23a}$$

$$Pe_{yy} = \frac{v_y \Delta y}{D_{yy}}, \tag{23b}$$

$$Pe_{xy} = \frac{(v_x v_y)^{0.5} (\Delta x \Delta y)^{0.5}}{D_{xy}}, \tag{23c}$$

$$Sr = k \Delta t. \tag{24}$$

The ratio of truncation terms to the corresponding physical terms can be expressed as a function of the dimensionless numbers.

$$\begin{aligned} \frac{D_{num,xx}}{D_{xx}} &= \frac{Pe_{xx}}{2} - \frac{5Sr}{4} - \frac{Pe_{xx}Sr}{4} + \frac{Pe_{xx}Cr_{xx}}{2} \\ &\quad - \sum_{m=2}^{\infty} \frac{(-1)^m}{(m-1)!} \left[-Sr^{m-1} + \frac{(m-1)}{2} Sr^{m-2} Pe_{xx} Cr_{xx} \right] \\ &\quad \times \left(1 + \frac{Sr}{2} + \frac{Sr}{2^{m+1}} \right) + \sum_{m=2}^{\infty} \frac{(-1)^m}{(m)!} \left(\frac{Sr}{2} \right)^{m-1} \\ &\quad \times \left[\frac{Sr}{2} + \frac{Sr Pe_{xx}}{4} - \frac{m Pe_{xx} Cr_{xx}}{2} \right], \end{aligned} \tag{25}$$

$$\begin{aligned} \frac{D_{num,yy}}{D_{yy}} &= \frac{Pe_{yy}}{2} - \frac{5Sr}{4} - \frac{Pe_{yy}Sr}{4} + \frac{Pe_{yy}Cr_{yy}}{2} \\ &\quad - \sum_{m=2}^{\infty} \frac{(-1)^m}{(m-1)!} \left[-Sr^{m-1} + \frac{(m-1)}{2} Sr^{m-2} Pe_{yy} Cr_{yy} \right] \\ &\quad \times \left(1 + \frac{Sr}{2} + \frac{Sr}{2^{m+1}} \right) + \sum_{m=2}^{\infty} \frac{(-1)^m}{(m)!} Sr^{m-1} \\ &\quad \times \left[\frac{Sr}{2} + \frac{Sr Pe_{yy}}{4} - \frac{m Pe_{yy} Cr_{yy}}{2} \right], \end{aligned} \tag{26}$$

$$\begin{aligned} \frac{D_{num,xy}}{D_{xy}} &= -3Sr + Pe_{xy} Cr_{xy} - \sum_{m=2}^{\infty} \frac{(-1)^m}{(m-1)!} \\ &\quad \times [-2Sr^{m-1} + (m-1)Sr^{m-2} Pe_{xy} Cr_{xy}] \\ &\quad \times \left(1 + \frac{Sr}{2} + \frac{Sr}{2^{m+1}} \right) + \sum_{m=2}^{\infty} \frac{(-1)^m}{(m)!} \left[\left(\frac{Sr}{2} \right)^m + Sr^m \right] \\ &\quad - \frac{1}{2} \sum_{m=2}^{\infty} \frac{(-1)^m}{(m-1)!} Pe_{xy} Cr_{xy} \left[\left(\frac{Sr}{2} \right)^{m-1} + Sr^{m-1} \right], \end{aligned} \tag{27}$$

$$\begin{aligned} \frac{v_{num,x}}{v_x} &= -\frac{5Sr}{4} + \frac{1}{2} \sum_{m=2}^{\infty} \frac{(-1)^m}{(m-1)!} \left[\left(\frac{Sr}{2} \right)^m + Sr^m \right] \\ &\quad + \sum_{m=2}^{\infty} \frac{(-1)^m}{(m)!} \left(\frac{Sr}{2} \right)^m, \end{aligned} \tag{28}$$

$$\frac{v_{num,y}}{v_y} = -\frac{5Sr}{4} + \frac{1}{2} \sum_{m=2}^{\infty} \frac{(-1)^m}{(m-1)!} \left[\left(\frac{Sr}{2} \right)^m + Sr^m \right] + \sum_{m=2}^{\infty} \frac{(-1)^m}{(m)!} Sr^m, \tag{29}$$

$$\frac{k_{num}}{k} = -\frac{3Sr}{4} + \frac{1}{2} \sum_{m=2}^{\infty} \frac{(-1)^m}{m!} \left[\left(\frac{Sr}{2} \right)^m + Sr^m \right]. \tag{30}$$

As seen, the second-order truncation error or numerical dispersion has three expressions, two expressions in X , Y directions and one cross-term expression. The second-order truncation error is a function of Pe , Cr and Sr numbers. We present new numerical dispersion ($D_{num,xy}$, cross-term numerical dispersion) that introduces new dimensionless numbers as Pe_{xy} and Cr_{xy} . As seen, cross-numerical dispersion ($D_{num,xy}$) exists even for the cases of zero physical dispersion, similar for the directional dispersions. This subject is important when physical dispersion is small or negligible (in many numerical solutions of contaminant transport equation in multi-dimensions, cross-term of physical dispersion is ignored) then numerical dispersion becomes a serious problem, leading to smearing of concentration fronts, so $D_{num,xy}$ should be considered for improvement of result. The first-order truncation error has two expressions in X and Y directions and they are functions of Sr only. Zero-order truncation error has only one component and it is function of Sr .

If the same approach is used for other FDM schemes, we can formulate truncation errors in general form, for all FD schemes in one-, two- or three-dimensional ADRE as

$$\left\{ \begin{aligned} \frac{D_{num,x_j x_j}}{D_{x_j x_j}} &= -\frac{4\omega Sr}{(1 + \delta_{ij})} + \delta_{ij} \left(\frac{1}{2} - \alpha_i \right) Pe_{x_i x_j} \\ &\quad + \delta_{ij} \left(\alpha_i - \frac{1}{2} \right) \omega Sr Pe_{x_i x_j} + \omega Pe_{x_i x_j} Cr_{x_i x_j} \\ &\quad - \sum_{m=2}^{\infty} \frac{(-1)^m}{(m-1)!} [-2Sr^{m-1} \\ &\quad + (m-1)Sr^{m-2} Pe_{x_i x_j} Cr_{x_i x_j}] \frac{(1 + \omega Sr)}{(1 + \delta_{ij})} \\ &\quad - \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} Sr^{m-1} Pe_{x_i x_j} Cr_{x_i x_j} \right] \omega \\ &\quad + \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m)!} \frac{2}{(1 + \delta_{ij})} Sr^m \right] \\ &\quad \times \left(1 - \alpha_i Pe_{x_i x_j} + \delta_{ij} \frac{Pe_{x_i x_j}}{2} \right) \omega, \\ \delta_{ij} &= \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}, \quad i, j = 1, 2, 3, \end{aligned} \right. \tag{31}$$

$$\frac{v_{\text{num}x_i}}{v_{x_i}} = -2\omega Sr + \sum_{m=2}^{\infty} \left[\frac{(-1)^m Sr^{m-1}}{(m-1)!} \right] (1 + \omega Sr) + \sum_{m=2}^{\infty} \left[\frac{(-1)^m Sr^m}{(m)!} \right] \omega, \quad (32)$$

$$\frac{k_{\text{num}}}{k} = -\omega Sr + \sum_{m=2}^{\infty} \left[\frac{(-1)^m Sr^{m-1}}{m!} \right] (1 + \omega Sr). \quad (33)$$

It should be noted that term Sr^{m-2} in Eq. (31) has been considered equal one, when $Sr = 0.0$ and $m = 2$. Also based on the comparison between Peclet and Courant numbers in one- and two-dimensions, we can define these dimensionless numbers in general form as

$$Pe_{x_i x_j} = \frac{(v_{x_i} v_{x_j})^{0.5} (\Delta x_i \Delta x_j)^{0.5}}{D_{x_i x_j}}, \quad (34)$$

$$Cr_{x_i x_j} = \frac{(v_{x_i} v_{x_j})^{0.5} (\Delta t)}{(\Delta x_i \Delta x_j)^{0.5}}. \quad (35)$$

To use above equation, it should be noted that parameters α_i , and ω for different schemes are defined as follows:

1. explicit approximation, upstream weighting with positive velocity ($\omega = 0.0$, $\alpha_i = 0.0$ with $u_i > 0$);
2. explicit approximation, central in distance ($\omega = 0.0$, $\alpha_i = 0.5$);
3. Crank–Nicolson approximation, upstream weighting with positive velocity ($\omega = 0.5$, $\alpha_i = 0.0$);
4. Crank–Nicolson approximation, central in distance ($\omega = 0.5$, $\alpha_i = 0.5$);
5. implicit approximation, upstream weighting with positive velocity ($\omega = 1.0$, $\alpha_i = 0.0$ with $u_i > 0$);
6. implicit approximation, central in distance ($\omega = 0.5$, $\alpha_i = 0.5$).

The variation of the ratio of numerical dispersion term to principal-term of physical dispersion (D_{num}/D) versus Sr are illustrated in Fig. 1 for four discretization schemes: (a) implicit upstream; (b) Crank–Nicolson upstream; (c) explicit upstream; and (d) ADI upstream method. This ratio for $D_{\text{num}yy}/D_{yy}$ and $D_{\text{num}xy}/D_{xy}$ has same behavior. Fig. 1 is obtained based on Eq. (31). Results in Fig. 1 demonstrate the variation in numerical dispersion from one discretization to another as function of Sr for three Peclet and Courant numbers; 1, 5, 10.

These results demonstrate that as the Pe number increases the absolute value of numerical dispersion increases. Increasing the Courant number leads to an increase in the absolute value of numerical dispersion in explicit and implicit upstream schemes and a decrease in numerical dispersion for ADI method. For the case of Crank–Nicolson scheme, the absolute value of numerical dispersion increases in some cases and de-

creases in some others. Also numerical dispersion decreases as the Sr increases for explicit, implicit and ADI schemes. Fig. 1 shows that zero numerical dispersion can be obtained with some specific values of Sr , Pe , and Cr , e.g. upstream explicit approximation with $Cr = 1.0$ and upstream Crank–Nicolson scheme with $Sr = 0.2$ and $Cr = 10.0$ have zero numerical dispersion.

From stability criteria for reaction term, Sink/Source number (Sr) cannot be greater than 1 [11]. Also it is not possible physically that Sr to be greater than 1, because all concentration is removed at one step. So in Figs. 1 and 2 Sr is limited to 1.0. The stability criteria for the advection term in explicit methods, limits the Courant number to 1.0, therefore explicit method for $Cr = 5$, 10 is unstable and the shown results for this case with $Cr = 5$, 10 are only provided for the sake of comparison with other given results in Fig. 1.

Implicit and ADI methods show similar behavior with respect to Sr , Pe , and Cr but ADI method has a very low numerical dispersion under all condition in comparison to explicit and implicit methods and its numerical dispersion is similar to Crank–Nicolson method.

So Crank–Nicolson and ADI methods are more accurate than other methods. Also Crank–Nicolson and ADI methods have a very low numerical dispersion in comparison with other two methods even for the advection-dominated problems (for large values of Pe and Cr numbers). Explicit and implicit methods introduce a very large value of numerical dispersion in the vicinity of $Sr = 0.0$. Fig. 1 shows that numerical dispersion for explicit method has negative value and has positive value for implicit and ADI methods. Numerical dispersion has both negative and positive values for Crank–Nicolson scheme.

For a given velocity, v , and dispersion coefficient, D , the value of the Peclet number is controlled only by the size of grid spacing (Δx or Δy). The Courant number is inversely proportional to the grid spacing, therefore, reducing the grid spacing results in an increase in the Courant number. Fig. 1 illustrates that the numerical dispersion is more sensitive to variations of Peclet number rather than the variations of Courant number.

Eq. (32) (first-order truncation error) is described in Fig. 2 for the same four discretization schemes (implicit, explicit, Crank–Nicolson and ADI upstream methods). Fig. 2 demonstrates the variation in numerical velocity. The absolute value of numerical velocity increases (numerical velocity has positive value for explicit method and has negative value for implicit and ADI methods) as the Sr increases (and reaches to 60% of actual velocity at $Sr = 1.0$) for explicit, implicit and ADI methods but, comparatively Crank–Nicolson scheme does not show any considerable changes in numerical velocity with increasing Sr and it is approximately equal zero.

Numerical reaction coefficient, Eq. (33), is illustrated in Fig. 3. It shows that zero-order reaction coefficient

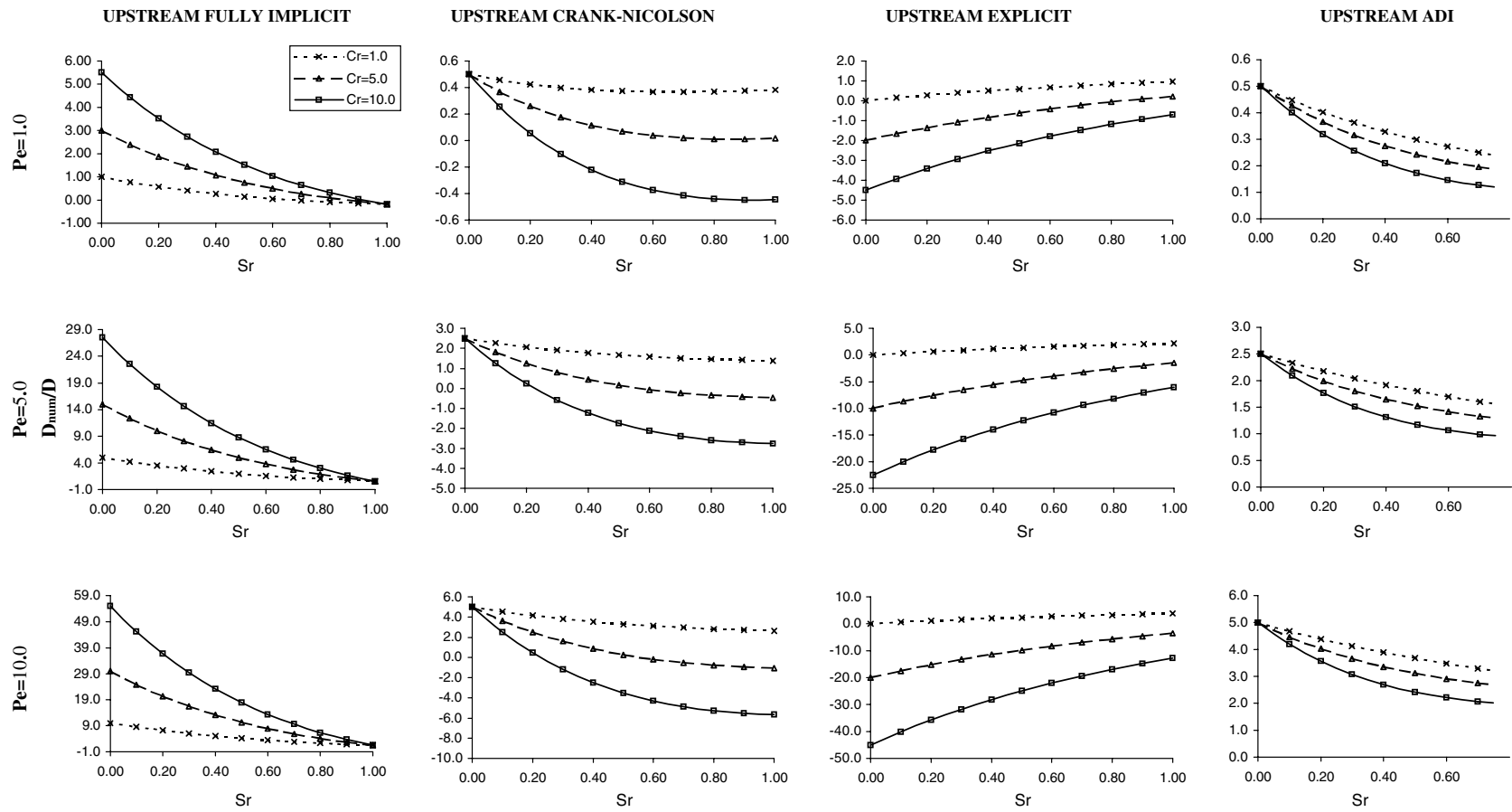


Fig. 1. Ratio of principal term of numerical dispersion coefficient to principal term of physical dispersion coefficient for different schemes (D_{num}/D).

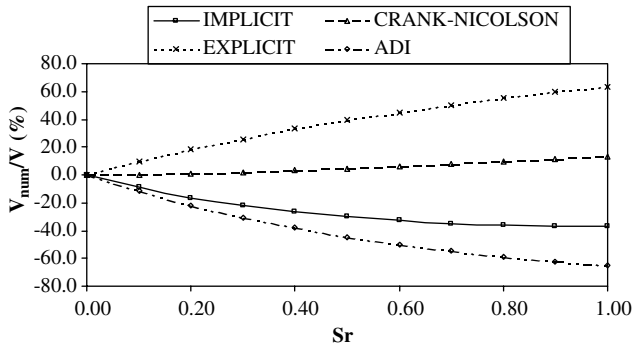


Fig. 2. Ratio of numerical velocity to physical velocity (V_{numx}/V_x or V_{numy}/V_y).

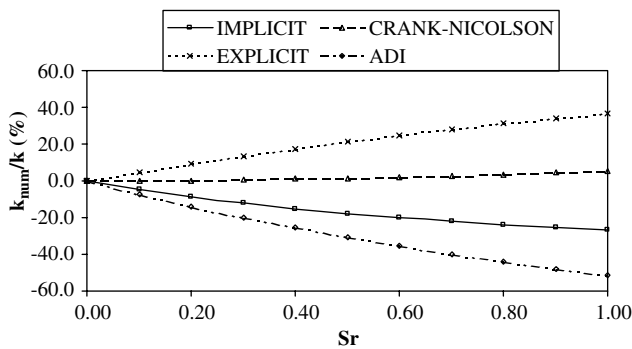


Fig. 3. Ratio of numerical reaction coefficient to physical reaction coefficient (k_{num}/k).

increases as Sr increases for explicit, implicit and ADI schemes but, considerable changes in numerical reaction occurs in ADI method and low changes for Crank–Nicolson method in comparison with the other two methods. Comparing Figs. 2 and 3 show that the first- and zero-order truncation errors have a similar behavior. Figs. 2 and 3 show that first- and zero-order truncation errors can be ignored if Sink/Source number becomes nearly zero. So if time step for numerical solution was chosen small as much as possible or reaction coefficient was small then the first- and zero-order truncation errors can be ignored.

As shown, there is a zero-order truncation error term in this form of equation, K_{num} . Therefore, even the mass balance of numerical solution does not maintained. As shown, by Ataie-Ashtiani et al. [4] for the one-dimensional ADRE, Crank–Nicolson scheme does not have second-order accuracy for ADRE generally. However, still it is a very accurate scheme considering the second-, first-, and zero-order truncation errors.

5. Removing truncation errors

The possibility of estimating truncation errors, has led to approaches in which a correction term equal

and opposite to numerical coefficient is added to physical coefficient [4,29]. The influence of truncation errors on the results of the numerical solution by ADI method is studied here. To remove the induced numerical truncation errors from the upstream ADI finite difference model, Eq. (12) is rewritten as [4,29]:

$$\begin{aligned} \frac{C_{i,j}^{n+1/2} - C_{i,j}^n}{\Delta t/2} = & D_{xx1}^* \left[\frac{C_{i+1,j}^{n+1/2} - 2C_{i,j}^{n+1/2} + C_{i-1,j}^{n+1/2}}{\Delta x^2} \right] \\ & + D_{yy1}^* \left[\frac{C_{i,j+1}^n - 2C_{i,j}^n + C_{i,j-1}^n}{\Delta y^2} \right] \\ & + D_{xy1}^* \left[\frac{C_{i+1,j+1}^{n+1/2} - C_{i+1,j-1}^{n+1/2} - C_{i-1,j+1}^{n+1/2} + C_{i-1,j-1}^{n+1/2}}{2\Delta x\Delta y} \right] \\ & - V_{x1}^* \left[\frac{C_{i,j}^{n+1/2} - C_{i-1,j}^{n+1/2}}{\Delta x} \right] \\ & - V_{y1}^* \left[\frac{C_{i,j}^n - C_{i,j-1}^n}{\Delta y} \right] - k^* C_{i,j}^{n+1/2}, \end{aligned} \quad (36)$$

where marked with asterisk terms are corrected coefficient:

$$\begin{aligned} D_{xx1}^* &= D_{xx} - D_{numxx1}, & D_{yy1}^* &= D_{yy} - D_{numyy1}, \\ D_{xy1}^* &= D_{xy} - D_{numxy1}, & v_{x1}^* &= v_x - v_{numx1}, \\ v_{y1}^* &= v_y - v_{numy1}, & k^* &= k - k_{num}. \end{aligned}$$

And for step (2) we will have:

$$\begin{aligned} \frac{C_{i,j}^{n+1} - C_{i,j}^{n+1/2}}{\Delta t/2} = & D_{xx2}^* \left[\frac{C_{i+1,j}^{n+1/2} - 2C_{i,j}^{n+1/2} + C_{i-1,j}^{n+1/2}}{\Delta x^2} \right] \\ & + D_{yy2}^* \left[\frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{\Delta y^2} \right] \\ & + D_{xy2}^* \left[\frac{C_{i+1,j+1}^{n+1} - C_{i+1,j-1}^{n+1} - C_{i-1,j+1}^{n+1} + C_{i-1,j-1}^{n+1}}{2\Delta x\Delta y} \right] \\ & - V_{x2}^* \left[\frac{C_{i,j}^{n+1/2} - C_{i-1,j}^{n+1/2}}{\Delta x} \right] - V_{y2}^* \left[\frac{C_{i,j}^{n+1} - C_{i,j-1}^{n+1}}{\Delta y} \right] \\ & - k^* C_{i,j}^{n+1}, \end{aligned} \quad (37)$$

where

$$\begin{aligned} D_{xx2}^* &= D_{xx} - D_{numxx2}, & D_{yy2}^* &= D_{yy} - D_{numyy2}, \\ D_{xy2}^* &= D_{xy} - D_{numxy2}, & v_{x2}^* &= v_x - v_{numx2}, \\ v_{y2}^* &= v_y - v_{numy2}, & k^* &= k - k_{num}. \end{aligned}$$

The effect of zero-, first- and second-order truncation errors on the results of ADI upstream FD scheme is assessed by comparing the FD model results with the analytical solution for a two-dimensional solute transport case with continuous point source. A large collection of analytical solutions for solute transport is

available in literature [30]. Solutions for one-dimensional solute-transport equation for variety of boundary and initial conditions are given in Van Genuchte and Alves [31]. Fewer analytical solutions have been published for the two- and three-dimensional forms of the solute transport equation. Wexler [32] gathered analytical solutions for advective–dispersive solute-transport equation with a variety of aquifer and solute-source configurations and boundary conditions in systems having uniform (unidirectional) ground water flow. In uniform flow, it is possible to align an axis (say the x axis) with the direction of the velocity vector so that: $v_x = v$, $v_y = 0$. In this case the cross-terms D_{xy} and D_{yx} are equal to zero.

The analytical solutions of the continuous point source problems have been presented by several authors [32–34]. Solving the ADRE for an instantaneous point source and then integrating the solution over the time obtain the solution. The two-dimensional ADRE for a continuous point source in uniform groundwater flow, modified from Wexler [32], is given by

$$\frac{\partial C}{\partial t} = D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{yy} \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} - kC + \frac{Q'}{nA} C_0 \delta(x - X_c) \delta(y - Y_c). \quad (38)$$

The analytical solution for Eq. (38) is given for the following initial and boundary conditions.

Boundary conditions:

$$C = 0, \quad \frac{\partial C}{\partial y} = 0, \quad y = \pm\infty, \quad (39a)$$

$$C = 0, \quad \frac{\partial C}{\partial x} = 0, \quad x = \pm\infty. \quad (39b)$$

Initial condition:

$$C = 0, \quad -\infty < x < \infty \text{ and } -\infty < y < +\infty \text{ at } t = 0, \quad (40)$$

where, v is velocity [LT^{-1}], Q' is fluid injection rate per unit thickness of aquifer [L^2T^{-1}], n is aquifer porosity [-], δ is Dirac delta (impulse) function, X_c , Y_c are x and y coordinates of point source [L], A is area of discretization cell at point source [L^2], C_0 is solute concentration in injected fluid [ML^{-3}].

The assumptions for analytical solution are

1. Fluid is of constant density and viscosity;
2. Flow in x -direction only, and velocity is constant;
3. Longitudinal and transverse dispersion coefficient (D_{xx}, D_{yy}) are constant.

The following equation represent analytical solution for an instantaneous point source integrated with respect to time [33] such that:

$$C(x,y,t) = \frac{C_0 Q'}{4n\pi\sqrt{D_{xx}D_{yy}}} \exp\left[\frac{v(x-X_c)}{2D_{xx}}\right] \int_0^t \frac{1}{\tau} \times \exp\left[-\left(\frac{v^2}{4D_{xx}} + k\right)\tau - \frac{(x-X_c)^2}{4D_{xx}\tau} - \frac{(y-Y_c)^2}{4D_{yy}\tau}\right] d\tau, \quad (41)$$

where τ is dummy variable of integration for the time integral.

A square media is considered for modeling and the parameters are given in Table 1. This problem is solved with $\Delta x = 50.0$ mm, $\Delta y = 50.0$ mm, and $\Delta t = 20.0$ s. The position of point source is $X_c = 0.0$ mm and $Y_c = 5000.0$ mm. The dimensionless numbers for this problem Pe_{xx} , Pe_{xy} , Pe_{yy} , Cr_{xx} , Cr_{xy} , Cr_{yy} , and Sr are 1.67, 0.0, 0.0, 0.8, 0.0, 0.0, and 0.01, respectively.

Concentration distribution and 10 contour levels of C/C_0 (between 0.02 and 0.2) in X – Y plane are shown in Fig. 4. As shown, the difference between numerical and analytical solution becomes larger as getting far from the point source to the front of plume. Two points, A and B (Fig. 4), are considered at each side of plume and time series of concentration for points A and B is illustrated in Figs. 5 and 6. As seen, the predicted numerical solution of concentration is more accurate for the case with correction for truncation errors. If the absolute value of errors is calculated at each node in the domain of solution, the differences between numerical solution with and without correction are better understood. The total or cumulative absolute value of errors is considered to be the summation of the absolute value of differences between nodal values of the analytical and numerical solutions.

The cumulative absolute value of errors with and without correction is shown in Fig. 7 for different times. The cumulative absolute value of errors after 500.0 s, without correction is 960 mg l^{-1} . This value reduces to 282 mg l^{-1} when the correction is applied. This case shows that the corrections for truncation errors are

Table 1
Parameter value used in ADRE

Property	Units	Value
Longitudinal velocity, v_x	mm s ⁻¹	2
Transverse velocity, v_y	mm s ⁻¹	0
Solute concentration in injected fluid, C_0	mg l ⁻¹	1000
First-order reaction coefficient, k	h ⁻¹	2
Longitudinal grid spacing, Δx	mm	50
Transverse grid spacing, Δy	mm	50
Time step, Δt	s	20
Longitudinal dispersion coefficient, D_{xx}	mm ² s ⁻¹	60
Transverse dispersion coefficient, D_{yy}	mm ² s ⁻¹	36
Cross term dispersion coefficient, D_{xy}	mm ² s ⁻¹	0
Fluid injection per unit thickness, Q'	mm ² s ⁻¹	12.5
Porosity, n	–	0.25

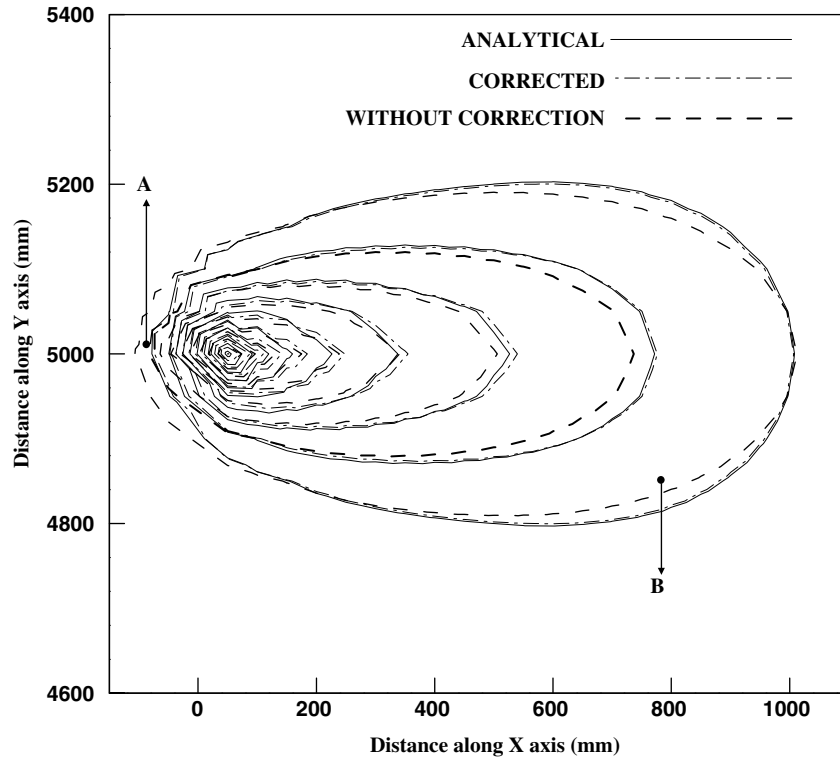


Fig. 4. Concentration distribution and contour levels of continuo point source from analytical and numerical solution after 500.0 s.

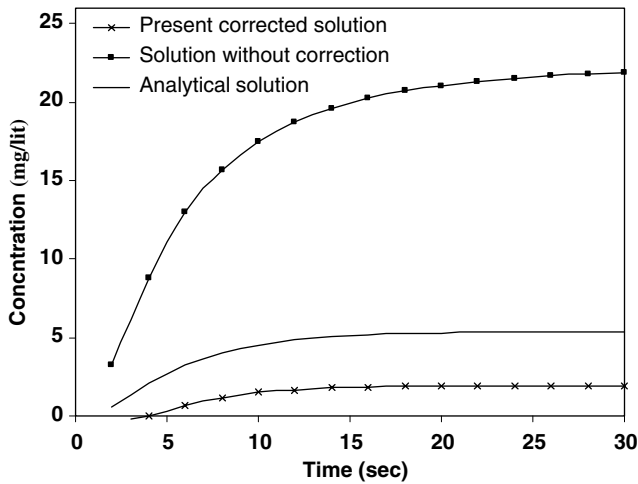


Fig. 5. Concentration variation for point A at different times.

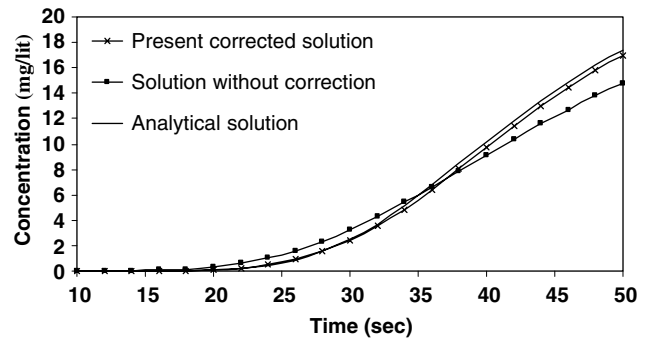


Fig. 6. Concentration variation for point B at different times.

quiet effective in improving the results of numerical solution by the ADI scheme.

Although Figs. 4–7 show a significant improvement in the numerical results, it should be noted that there are other kind of errors such as round-off that cannot be removed by the provided method. More importantly, it also should be considered that in any case all the of the truncation errors cannot be removed as we do not have the third- and higher-order spatial derivatives in the equations and therefore these truncated terms cannot be corrected in this approach.

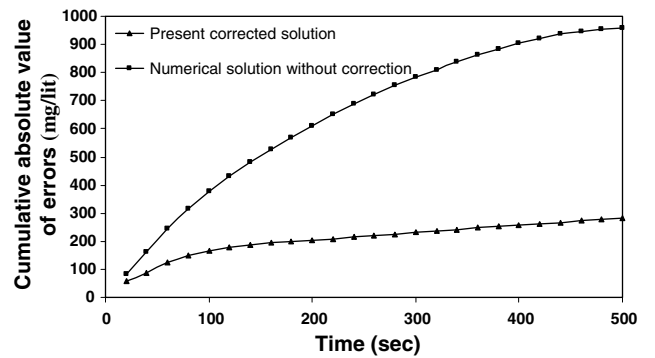


Fig. 7. Cumulative absolute value of errors for numerical solution with and without correction.

6. Conclusion

There are many numerical investigations of the advection–dispersion equation. However, comparatively few studies have been devoted to the more general advection–dispersion–reaction equation. This equation is practically important because the governing equation of many cases fall into this category. In this work, the expressions for the truncation errors associated with the finite difference solution of two-dimensional advection–dispersion equation with first-order reaction or degradation are obtained in general. These truncation errors are presented as function of principal and cross-terms of Peclet and Courant numbers and Sink/Source dimensionless numbers. The numerical dispersion is a function of Peclet, Courant, and Sink/Source numbers. In fact the Sink/Source number has a significant effect on the magnitude of numerical dispersion.

It is shown that widely used finite difference schemes have low-order truncation errors for the ADRE, even the Crank–Nicolson approximation scheme. In fact, none of these methods has even zero-order accuracy for ADRE.

The variation of these truncation errors is illustrated as function of Peclet, Courant, and Sink/Source numbers for explicit, implicit, Crank–Nicolson and ADI upstream methods. Results show none of these methods is free of truncation errors and only for some specific values of Pe , Cr , and Sr numerical dispersion is zero. Principal and cross-terms of numerical dispersion increase with the increase of Peclet number. This trend is inversely observed as Sink/Source number increases in general except for Crank–Nicolson method. Moreover, absolute value of numerical velocity and numerical reaction term increase with increase in Sink/Source number, while Crank–Nicolson scheme has lowest numerical velocity and numerical reaction among these schemes.

The effect of these truncation errors on the solution of two-dimensional advection–dispersion equation with first-order reaction term is demonstrated for a case with a known analytical solution in uniform flow field. Advection–dispersion–reaction equation in two dimensions was solved with alternating direction implicit method. Comparison shows that these errors are not negligible and disturb mass balance in numerical solution. Removing these errors can significantly improve the numerical result and produces a more accurate numerical solution; also, it is possible to solve practical problems by sufficiently increasing the time or depth increment without numerical oscillation or artificial oscillation.

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