Chapter 18
Numerical Errors Associated with Groundwater Models and Improving the Reliability of Models in Environmental Management Issues

K. V. Sruthi, Kim Hyun Su, Anupma Sharma and N. C. Ghosh

Abstract Improving numerical accuracy of the finite difference (FD) models of groundwater transport is achieved here by removing the truncation error associated with advection–dispersion equation with first-order reaction and sink/source (ADERS). This chapter presents theoretical and numerical truncation error associated with ADERS for the first time. The truncation errors associated with the FD models of the ADERS are formulated from Taylor series analysis. The error expressions are based on a general form of the corresponding FD equation. A temporally and spatially weighted parametric approach is applied to differentiate among the various FD models. The study revealed that all the FD models (explicit, Crank–Nicolson, implicit) suffer from truncation errors and formulated an expression for error from sink/source term for the first time. The effects of these truncation errors on the solution of ADERS are demonstrated by comparison of numerical solution from different FD models with the analytical solution. The results revealed that these errors are not negligible and correcting the FD schemes for truncation error can result in a more accurate solution in groundwater transport models which are applied for environmental management as well as hydrological investigations.

Keywords Truncation error · Finite difference method · ADERS subsurface transport models · Numerical accuracy

---

K. V. Sruthi (✉) · A. Sharma · N. C. Ghosh
Groundwater Hydrology Division, National Institute of Hydrology, Roorkee, Uttarakhand, India
e-mail: kvsruthi@gmail.com

K. V. Sruthi
KSCSTE—Centre for Water Resources Development and Management, Kozhikode, Kerala, India

K. H. Su
Department of Earth and Environmental Sciences, Chonbuk National University, Jeonju, Republic of Korea

The Earth and Environmental Science System Research Center, Chonbuk National University, Jeonju, Republic of Korea

R. M. Singh et al. (eds.), *Environmental Processes and Management*,
Water Science and Technology Library 91,
https://doi.org/10.1007/978-3-030-38152-3_18

18.1 Introduction

Mathematical models play a major role in describing the contamination of groundwater and soil water which are widely recognized as most critical environmental problems of recent times. The emergence of this notion witnessed the development of an increasing number of mathematical models (MODFLOW, MT3DMS, FEFLOW, PHT3D) describing the flow and transport processes of groundwater. These models are used as tools for decision making in the management of a water resource system. They may also be used to predict future groundwater scenarios. Therefore, groundwater models are now an important part of many hydrogeological investigations.

An equation describing a groundwater transport model is a partial differential equation (advection–dispersion equation, ADE). It can be solved mathematically by analytical or numerical solutions. Analytical solutions are very difficult to apply because they require specific parameters and boundaries that should be highly idealized. Therefore, numerical models are used in groundwater modeling as it yields approximate solutions to the governing equations through discretization of space and time. One of the main types of numerical models that are accepted for solving the groundwater transport equation is the finite difference method (FDM), an approach to computational fluid dynamics (CFD) and very effective in groundwater modeling (Anderson and Woessner 1992; Igboekwe et al. 2008). In this method, continuous variable is replaced by discrete variables that are defined at grid blocks. Also, the continuous differential equations which define the variable in the system are replaced by a finite number of variables at different grids. Ultimately, FDM seems to be more popular to solve ADE mainly due to the ease of implementation and its relative simplicity (Ataie-Ashtiani et al. 1999a, b; Sheu et al. 2000).

In all of these applications, an understanding of model accuracy is essential. Several approaches have been developed previously in order to improve the numerical accuracy of the models. One factor affecting the accuracy of the FDM is the numerical error, which occurs in all computational simulations. Numerical error can lead to quantitative and even qualitative changes in simulation results, potentially affecting the management of field sites (Simmons et al. 1999; Woods et al. 1998, 1999). There are many types of numerical errors. For instance, if the chosen grid spacing and time step length are too large, small errors may grow to dominate part of that simulation, resulting in numerical instability (Ferziger and Perić 1999; Noye 1978). This often leads to physically unreasonable results and problems with convergence. Another kind of numerical error is the truncation error (Gresho and Sani 1998; Noye and Hayman 1985). Approximating differential equations in the FDM by discretization introduces truncation error. Truncation error limits the use of numerical finite difference approximations in order to solve the partial differential equations. In case of ADE, numerical dispersion is the well-known consequence of truncation error. It results in an artificial dispersion, velocity, reaction term often denoted as numerical diffusion, numerical velocity, and numerical reaction coefficient. Numerical dispersion is insidious because it mimics the hydrodynamic dispersion (heuristic description of various physical processes) (Bear 1972) producing smooth results that may seem plausible.

In previous studies, truncation errors for the FDM were first evaluated theoretically and then spot-checked with numerical calculations (Lantz 1971). Chaudhari (1971) applied an explicit-backward space FDM and showed that the addition of a term to the dispersion coefficient could reduce the smearing of a front by generating non-oscillatory numerical solutions. This study quantified the numerical dispersion as a second-order error through the examination of the truncated Taylor series approximation of an explicit FD solution of one-dimensional ADE. Pinder and Gray (1977) adopted Fourier analysis to examine the behavior of the numerical error in time for FD schemes. Their work provided a valuable insight into the nature of numerical dispersion. Unfortunately, it did not yield easily applicable criteria for the control of numerical dispersion in real-world situations. Campbell et al. (1981) presented criteria for the control of numerical dispersion in a solution using the FD formulation for the time derivative. Several other schemes have been proposed in order to minimize the effects of numerical dispersion through the application of dispersion coefficient corrections in the transport equation (Bresler 1973; Chaudhari 1971; Lantz 1971; Van Genuchten and Wierenga 1974). Several studies have also considered the effect of numerical dispersion associated with the ADE during their simulations (May and Noye 1984; Noye 1990; Van Genuchten and Gray 1978).

Typically, the above-mentioned studies have considered the effect of numerical dispersion because it is the only truncation error in case of ADE (De Smedt and Wierenga 1977; Dudley et al. 1991; Moldrup et al. 1992, 1994a, b; Notodarmojo et al. 1991; Van Genuchten and Gray 1978). However, general transport equation should include truncation errors from all physical process terms such as advection, dispersion, reaction, and sink/source term. Ataie-Ashtiani et al. (1996) estimated the truncation error from dispersion, advection, and reaction which were termed as numerical dispersion, numerical velocity, and numerical reaction coefficient, respectively. A correction method for the numerical truncation errors of an explicit centered in space scheme was proposed (Ataie-Ashtiani et al. 1996). Also, zero- and first-order truncation errors in the ADE with reaction (ADER) were quantified for all widely applied numerical models (Ataie-Ashtiani et al. 1999a, b). Further, these studies were carried out in order to assess the effects of these truncation errors on the numerical solution of a two-dimensional advection–dispersion equation with a first-order reaction (Ataie-Ashtiani and Hosseini 2005a, b). For instance, the well-known groundwater modeling software 'MT3DMS' which is widely being used by the groundwater community (Zheng 1999), applied the standard FDM in order to solve the ADE, in which the FDM suffers truncation error. Therefore, it is very important to estimate the truncation error resulting from various physical process terms in the ADE in order to avoid the numerical inaccuracy in groundwater transport models based on FDM. However, the truncation errors arising due to the sink/source term (zero-order production) in the ADER have not been considered in the previous studies. In other words, no previous studies estimated the truncation error due to the sink/source term in the ADERS.

Therefore, we estimate the analytical expressions for all truncation errors resulting especially from the sink/source term for the general FD form of the ADERS. The numerical model section includes the development of different FD models by the elimination of truncation error followed by results and discussion. The study covers explicit, Crank–Nicolson, and implicit schemes to reveal that none of the widely used FD scheme models have complete accuracy. This chapter also aims to provide the user more than just a qualitative effect for the importance of truncation error for all terms such as dispersion, advection, reaction, and sink/source. In addition, we also present the numerical results after eliminating the truncation errors specifically resulting from the sink/source term, which improves the results of the FD models based on ADERS and can lead to a more accurate numerical solution.

18.2 Numerical Approach

In the field of geosciences, the partial differential equation describing one-dimensional transport of a solute with sink/source term through a homogeneous subsurface medium is

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} - kC + Q \tag{18.1}$$

where C is the solute concentration [ML^{-3}]; t is time [T]; x is the horizontal coordinate [L]; U is the Darcy flux [LT^{-1}]; D is the physical dispersion coefficient [L^2T^{-1}], Q is the sink/source term.

A general form of the FD model using ω and α as the temporal and spatial weighting parameters, respectively, can be expressed as

$$\begin{aligned}
\frac{C_i^{n+1} - C_i^n}{\Delta t} &= D\left[\omega\frac{C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}}{\Delta x^2} + (1-\omega)\frac{C_{i+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2}\right] \\
&\quad - U\left[\begin{aligned} &\omega\frac{(1-\alpha)C_i^{n+1} + \alpha C_{i+1}^{n+1} - (1-\alpha)C_{i-1}^{n+1} - \alpha C_i^{n+1}}{\Delta x} \\ &+(1-\omega)\frac{(1-\alpha)C_i^n + \alpha C_{i+1}^n - (1-\alpha)C_{i-1}^n - \alpha C_i^n}{\Delta x}\end{aligned}\right] \\
&\quad - k\left[\omega C_i^{n+1} + (1-\omega)C_i^n\right] + Q
\end{aligned} \tag{18.2}$$

where the superscript n refers to the time level; the subscript i refers to the node point, Δx is the spatial increment of grid [L] and Δt is the temporal increment [T]. Here, uniform time and space increment is applied.

A Taylor series expansion of C about any grid point is used to determine the form of the truncation errors (Chaudhari 1971; Lantz 1971). By neglecting the third- and higher-order spatial derivatives, the following formulations are obtained

$$C_i^{n+1} \approx C_i^n + \sum_{m=1}^{\infty} \frac{\Delta t^m}{m!} \frac{\partial^m C}{\partial t^m} \tag{18.3}$$

$$C_{i+1}^{n+1} \approx C_i^{n+1} + \Delta x \frac{\partial C^{n+1}}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C^{n+1}}{\partial x^2} \tag{18.4}$$

$$C_{i-1}^{n+1} \approx C_i^{n+1} - \Delta x \frac{\partial C^{n+1}}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C^{n+1}}{\partial x^2} \tag{18.5}$$

$$C_{i+1}^{n} = C_i^{n} + \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C}{\partial x^2} \tag{18.6}$$

$$C_{i-1}^{n} = C_i^{n} - \Delta x \frac{\partial C}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C}{\partial x^2} \tag{18.7}$$

18.2.1 Determine the Expression for C_i^{n+1} in Terms of Spatial Derivative

In order to change Eq. (18.3) in terms of a spatial derivative, the following formulations are applied. The second- and the higher-order temporal derivatives of C are written in terms of spatial derivatives using the differentiated form of Eq. (18.1) as the following

$$\frac{\partial^2 C}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial C}{\partial t}\right) = \frac{\partial}{\partial t}\left(D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} - kC + Q\right) \tag{18.8}$$

$$\frac{\partial^2 C}{\partial t^2} = D\frac{\partial^2}{\partial x^2}\left(\frac{\partial C}{\partial t}\right) - U\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial t}\right) - k\left(\frac{\partial C}{\partial t}\right) + \frac{\partial Q}{\partial t} \tag{18.9}$$

In order to express Eq. (18.9) only in spatial terms, the temporal terms are eliminated. For the elimination of temporal terms, Eq. (18.1) is substituted into Eq. (18.9) as the following

$$\begin{aligned} &= D\frac{\partial^2}{\partial x^2}\left(D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} - kC + Q\right) \\ &\quad - U\frac{\partial}{\partial x}\left(D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} - kC + Q\right) \\ &\quad - k\left(D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} - kC + Q\right) + \frac{\partial Q}{\partial t} \end{aligned} \tag{18.10}$$

The higher-order derivatives are neglected. Here, Q is considered as a constant value. Therefore, the spatial and temporal derivative terms of Q become zero.

$$\frac{\partial^2 C}{\partial t^2} \approx \left(U^2 - 2kD\right)\frac{\partial^2 C}{\partial x^2} + 2kU\frac{\partial C}{\partial x} + k^2 C - kQ \tag{18.11}$$

Similarly, the higher-order temporal derivative can be formulated as follows

$$\frac{\partial^3 C}{\partial t^3} = \left(-3kU^2 + 3k^2 D\right)\frac{\partial^2 C}{\partial x^2} - 3k^2 U\frac{\partial C}{\partial x} - k^3 C + k^2 Q \tag{18.12}$$

$$\frac{\partial^4 C}{\partial t^4} = \left(6k^2U^2 - 4k^3 D\right)\frac{\partial^2 C}{\partial x^2} + 4k^3 U\frac{\partial C}{\partial x} + k^4 C - k^3 Q \tag{18.13}$$

$$\frac{\partial^5 C}{\partial t^5} = \left(-10k^3U^2 + 5k^4 D\right)\left(\frac{\partial^2 C}{\partial x^2}\right) - 5k^4 U\frac{\partial C}{\partial x} - k^5 C + k^4 Q \tag{18.14}$$

From Eqs. (18.11), (18.12), (18.13), and (18.14), the following general formula could be generated, i.e. for $m \geq 2$

$$\begin{aligned}\frac{\partial^m C}{\partial t^m} \approx (-1)^m&\left(\frac{m(m-1)}{2}k^{m-2}U^2 - mk^{m-1}D\right)\frac{\partial^2 C}{\partial x^2}\\ &+ (-1)^m mk^{m-1}U\frac{\partial C}{\partial x} + (-1)^m k^m C\\ &+ (-1)^{m-1}k^{m-1}Q\end{aligned} \tag{18.15}$$

Therefore, Eq. (18.3) could be written as the following

$$\begin{aligned}C_i^{n+1} \approx C_i^n &+ \Delta t\frac{\partial C}{\partial t}\\ &+ \sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[\begin{array}{r}(-1)^m\left(\frac{m(m-1)}{2}k^{m-2}U^2 - mk^{m-1}D\right)\frac{\partial^2 C}{\partial x^2}\\ +(-1)^m mk^{m-1}U\frac{\partial C}{\partial x} + (-1)^m k^m C + (-1)^{m-1}k^{m-1}Q\end{array}\right]\end{aligned} \tag{18.16}$$

Similarly, the formula for C_{i+1}^{n+1} and C_{i-1}^{n+1} in terms of the spatial derivative could be written as the following

$$\begin{aligned}C_{i+1}^{n+1} = C_i^n &+ \Delta t\frac{\partial C}{\partial t}\\ &+ \sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[\begin{array}{r}(-1)^m\left(\frac{m(m-1)}{2}k^{m-2}U^2 - mk^{m-1}D\right)\frac{\partial^2 C}{\partial x^2}\\ +(-1)^m mk^{m-1}U\frac{\partial C}{\partial x} + (-1)^m k^m C + (-1)^{m-1}k^{m-1}Q\end{array}\right]\\ &+ \Delta x\frac{\partial C}{\partial x} + \Delta x\Delta t\left(-U\frac{\partial^2 C}{\partial x^2} - k\frac{\partial C}{\partial x}\right)\end{aligned}$$

$$+\Delta x\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[\begin{array}{r}(-1)^m mk^{m-1}U\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m k^m\dfrac{\partial C}{\partial x}\end{array}\right]$$
$$+\frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2}-\Delta t\frac{\Delta x^2}{2}k\frac{\partial^2 C}{\partial x^2}+\frac{\Delta x^2}{2}\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m k^m\frac{\partial^2 C}{\partial x^2}\right] \quad (18.17)$$

$$C_{i-1}^{n+1}=C_i^n+\Delta t\frac{\partial C}{\partial t}$$
$$+\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[\begin{array}{r}(-1)^m\left(\dfrac{m(m-1)}{2}k^{m-2}U^2-mk^{m-1}D\right)\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m mk^{m-1}U\dfrac{\partial C}{\partial x}+(-1)^m k^m C+(-1)^{m-1}k^{m-1}Q\end{array}\right]$$
$$-\Delta x\frac{\partial C}{\partial x}-\Delta x\Delta t\left(-U\frac{\partial^2 C}{\partial x^2}-k\frac{\partial C}{\partial x}\right)$$
$$-\Delta x\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[\begin{array}{r}(-1)^m mk^{m-1}U\dfrac{\partial^2 C}{\partial x^2}\\ +(-1)^m k^m\dfrac{\partial C}{\partial x}\end{array}\right]$$
$$+\frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2}-\Delta t\frac{\Delta x^2}{2}k\frac{\partial^2 C}{\partial x^2}+\frac{\Delta x^2}{2}\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m k^m\frac{\partial^2 C}{\partial x^2}\right] \quad (18.18)$$

Substitution of all the Taylor series expansion for C about any grid point in the finite discretized approximation of solute transport equation in order to estimate the truncation error will result in the following equation. By inserting Eqs. (18.6), (18.7), (18.16), (18.17), and (18.18) into Eq. (18.2), the final expression for $\frac{\partial C}{\partial t}$ would be obtained in the following form

$$\frac{\partial C}{\partial t}=\frac{\partial^2 C}{\partial x^2}\left\{\begin{array}{l}D-2D\omega\Delta tk+\left(\alpha-\dfrac{1}{2}\right)u\omega\Delta x\Delta tk+\left(\dfrac{1}{2}-\alpha\right)U\Delta x+U^2\omega\Delta t\\ +(-1-k\omega\Delta t)\left[\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m\left(\frac{(m-1)}{2}k^{m-2}U^2-k^{m-1}D\right)\right]\\ +(-U\omega)\left[\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}(-1)^m mk^{m-1}U\right]\\ +\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m k^m\right]*\left(\omega D-\alpha u\omega\Delta x+u\omega\frac{\Delta x}{2}\right)\end{array}\right\}$$
$$-\frac{\partial C}{\partial x}\left[\begin{array}{r}U-2U\omega\Delta tk\\ +U\omega\displaystyle\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}(-1)^m k^m+(1+k\omega\Delta t)\left(\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m k^{m-1}U\right)\end{array}\right]$$

$$- C\left[k - \omega\Delta t k^2 + (1 + k\omega\Delta t)\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{m!}(-1)^m k^m\right]$$
$$\left[Q - k\omega\Delta t Q + (-1 - k\omega\Delta t)\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{m!}(-1)^{m-1}k^{m-1}Q\right] \qquad (18.19)$$

18.2.2 Derivation of the Truncation Error Formula

By comparing the above Eq. (18.19) with the original governing Eq. (18.1), four forms of truncation errors due to discretization are observed. It can be formulated as follows

Second-order truncation error or numerical dispersion

$$D_{\text{num}} = -2D\omega\Delta t k + \left(\alpha - \frac{1}{2}\right)U\omega\Delta x\Delta t k + \left(\frac{1}{2} - \alpha\right)U\Delta x + U^2\omega\Delta t$$
$$+ (-1 - k\omega\Delta t)\left[\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m\left(\frac{(m-1)}{2}k^{m-2}U^2 - k^{m-1}D\right)\right]$$
$$+ (-U\omega)\left[\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}(-1)^m m k^{m-1}U\right]$$
$$+ \sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m k^m\right] * (\omega D - \alpha U\omega\Delta x + U\omega\frac{\Delta x}{2}) \qquad (18.20)$$

First-order truncation error or numerical water velocity

$$U_{\text{num}} = -2U\omega\Delta t k + \sum_{m=2}^{\infty}\left[\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m k^{m-1}U\right](1 + k\omega\Delta t)$$
$$+ \sum_{m=2}^{\infty}\left[\frac{\Delta t^m}{m!}(-1)^m k^m\right]U\omega \qquad (18.21)$$

Zero-order truncation error or numerical reaction coefficient

$$k_{\text{num}} = -\omega\Delta t k^2 + \left[\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{m!}(-1)^m k^m\right](1 + k\omega\Delta t) \qquad (18.22)$$

Sink/Source term truncation error

$$Q_{\text{num}} = -k\omega\Delta t Q + (-1 - k\omega\Delta t)\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{m!}(-1)^{m-1}k^{m-1}Q \tag{18.23}$$

The truncation error due to the sink/source term (Q_{num}) is quantified in the above Eq. (18.23). It is to be noted that no previous studies have attempted to quantify the error due to the sink/source term.

18.2.3 Reformulation of the Truncation Error Corrected Subsurface Transport Equation

In order to eliminate the truncation error due to the numerical dispersion, numerical velocity, numerical reaction coefficient, and the source/sink truncation, the derived formula for these terms will be subtracted from the physical dispersion, velocity, reaction coefficient, and the sink/source term. The resulting terms are inserted in Eq. (18.1)

$$\frac{\partial C}{\partial t} = D*\frac{\partial^2 C}{\partial x^2} - U*\frac{\partial C}{\partial x} - k*C + Q* \tag{18.24}$$

where $D*$, $U*$, $k*$, $Q*$ denotes the truncation error corrected forms.

$$D^* = D - D_{\text{num}} \tag{18.25}$$

$$U^* = U - U_{\text{num}} \tag{18.26}$$

$$k^* = k - k_{\text{num}} \tag{18.27}$$

$$Q^* = Q - Q_{\text{num}} \tag{18.28}$$

18.3 Results and Discussion

In order to study the effect of numerical error due to numerical truncation of Taylor series expansion (numerical dispersion, numerical velocity, numerical reaction coefficient, numerical sink/source term) on FD model such as explicit scheme, Crank–Nicolson scheme, and implicit scheme, the study compared the numerical simulation results of truncation error corrected and non- corrected scheme with analytical solution. The analytical solution is adopted from van Genuchten and Alves (1982). The analytical solution for solute transport equation for the following initial and boundary condition

$$C(x, 0) = C_i \quad t = 0 \ \ x > 0$$

$$C(0, t) = C_o \quad t > 0 \ \ x = 0$$

$$\frac{\partial C}{\partial x}(\infty, t) = 0$$

is given as

$$C(x, t) = \frac{Q}{k} + \left(C_i - \frac{Q}{k}\right)A(x, t) + \left(C_o - \frac{Q}{k}\right)B(x, t)$$

where C_i represents initial concentration of solute in transport medium $[ML^{-3}]$, C_o is incoming concentration $[ML^{-3}]$.

$$A(x, t) = \exp(-kt)\left\{1 - \frac{1}{2}\text{erfc}\left[\frac{x - Ut}{2(Dt)^{1/2}}\right] - \frac{1}{2}\exp\left(\frac{Ux}{D}\right)\text{erfc}\left[\frac{x + Ut}{2(Dt)^{1/2}}\right]\right.$$

$$B(x, t) = \frac{1}{2}\exp\left[\frac{(U - v)x}{2D}\right]\text{erfc}\left[\frac{x - vt}{2(Dt)^{1/2}}\right] + \frac{1}{2}\exp\left[\frac{(U + v)x}{2D}\right]\text{erfc}\left[\frac{x + vt}{2(Dt)^{1/2}}\right]$$

And

$$v = U\left(1 + \frac{4kD}{U^2}\right)^{1/2}.$$

18.3.1 *Comparison of Numerical Solution of Corrected and Non-corrected Truncation Error for Different FD Schemes with Analytical Solution*

In order to compare the accuracy of truncation error corrected FD models, a numerical problem is formulated. The numerical problem is composed of a semi-infinite column, where $U = 5$ cm/h; $D = 100$ cm^2/h; $k = 0.1$ h^{-1}; source concentration = 100 mg/L; incoming concentration = 1000.0 mg/L. Here, a space increment of 20 cm and temporal increment of 1.0 h are applied. And the study compared the numerical solution with analytical solution at time of 20 h. Also, arbitrary units can be used for the numerical parameters. Figure 18.1 displays the comparison between the numerical simulation results (truncation error corrected and non-corrected) and analytical solution of numerical problem for different FD models. The results include the correction of all truncation error terms associated with advection—dispersion equation with first-order reaction and zero-order production term. The comparison between the results shows that none of the explicit schemes have the numerical accuracy without truncation error correction (Fig. 18.1). The numerical results from Crank–Nicolson method show that the centered scheme in space has negligible truncation error compared to other methods. The analytical solution and simulation results (truncation error corrected and non-corrected) for Crank–Nicolson centered scheme well matched each other. In Fig. 18.2, numerical results of implicit scheme reveal that implicit upstream and centered scheme without truncation error correction deviates

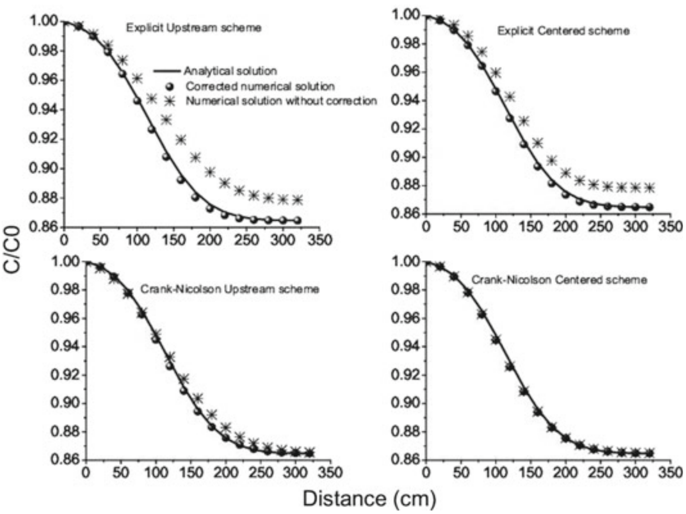

Fig. 18.1 Comparison of corrected and non-corrected numerical solution with analytical solution for explicit and Crank–Nicolson schemes with upstream and centered in space scheme

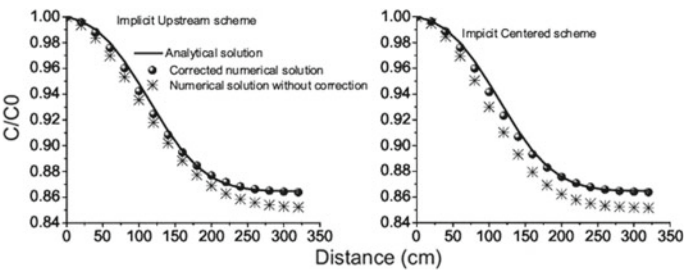

Fig. 18.2 Comparison of corrected and non-corrected numerical solution with analytical solution for implicit FD model with upstream and centered in space scheme

significantly from the analytical solution. The numerical results from truncation error corrected implicit scheme well corresponded with analytical solution (Fig. 18.2). From Figs. 18.1 and 18.2, it is absolutely clear that none of the FD models are free of truncation error; but the Crank–Nicolson centered scheme yields numerical solution which has negligible truncation error compared to other FD models.

18.3.2 *Estimation of Relative Error in the Numerical Results of Truncation Error Corrected and Non- Corrected FD Models*

The study estimated the relative error for truncation error corrected and non-corrected numerical solution of different FD models. Our results revealed that numerical error is decreased drastically by the removal of truncation error from FD models (Fig. 18.3). The maximum error limit is reduced from 3 to 0.5% after truncation error correction (Fig. 18.3). It is very significant to study the truncation error correction of FD model because the groundwater model such as MT3D applies FD models to solve the numerical problems. Application of truncation error correction term can reduce the error from numerical results of these FD models. The present study could shed light on the truncation error due to the advection term, dispersion, reaction term, and sink/source term. Especially, the study estimated for the first time a numerical formula for truncation error from sink/source term (Q_{num}).

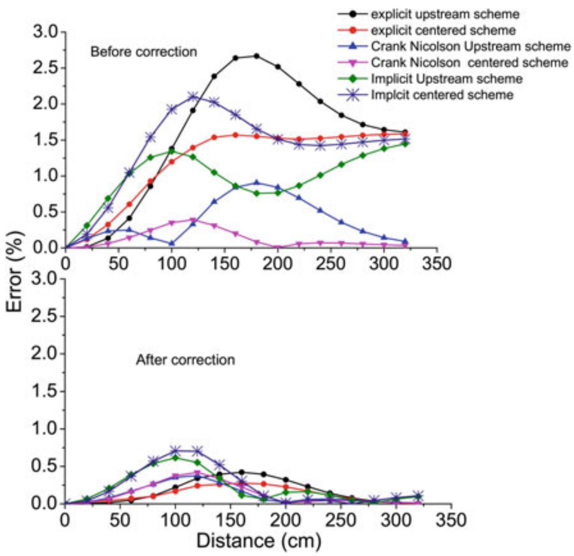

Fig. 18.3 Comparison of estimated error in numerical solution for different FD model before and after removal of truncation error

The present study reveals the importance of the removal of truncation error due to the different terms in ADERS. The study estimates the truncation error resulting from sink/source term and its effect on numerical accuracy of different FD models. It is revealed that numerical truncation error correction has a significant impact on improving solution accuracy of the finite difference models. Also, the numerical solution without error correction has shown a significant deviation from analytical solution in the case of all finite difference models except Crank–Nicolson-centered scheme. It showed a less deviation, even in the absence of truncation error correction. Here, the study estimates for the first time the truncation error term due to sink/source part in advection–dispersion equation. None of the studies have quantified the truncation error due to the sink/source term. Ultimately, the study reveals that none of the finite difference models are free of truncation error and the numerical accuracy is affected by several truncation errors which result from advection, dispersion, reaction, and sink/source term.

18.4 Conclusions

This chapter explains the estimation of the truncation error associated with the FDM models based on ADERS by applying the Taylor series expansion. The study analyzes the truncation error both theoretically and numerically. It reveals that modification or subtraction of numerical truncation error term significantly increases the solution accuracy of the FD model which is being applied widely in popular subsurface transport models such as MODFLOW, MT3DMS. Moreover, the study estimates the truncation error due to the sink/source term in the ADERS for the first time. The study compared the solution accuracy of the FD models with and without truncation error correction. The results showed that none of the FD models were free of truncation errors which ultimately lead to misinterpretation during hydrological investigations by affecting the accuracy. Here, the least truncation error was exhibited by Crank–Nicolson-centered scheme. Also, the study estimated the error in the numerical solution (both with correction and without correction), and it was observed that the maximum level of relative error reduced from 3 to 0.5% by eliminating the truncation error. The comparative study of numerical solution of FD models revealed that the truncation error correction can improve the solution accuracy of the FD models significantly. We suggest from this study that the application of truncation error removal method is most significant to increase the solution accuracy in different FD models, which is widely applied in the groundwater community.

Acknowledgements We would like to thank the Director, National Institute of Hydrology, Roorkee, India for constant encouragement and support.

References

Anderson MP, Woessner WW (1992) Applied groundwater modeling. Academic Press, San Diego, C. A, Simulation of Flow and Advective Transport

Ataie-Ashtiani B, Lockington D, Volker R (1996) Numerical correction for finite-difference solution of the advection–dispersion equation with reaction. J Contam Hydrol 23:149–156

Ataie-Ashtiani B, Volker R, Lockington D (1999a) Numerical and experimental study of seepage in unconfined aquifers with a periodic boundary condition. J Hydrol 222:165–184

Ataie-Ashtiani B, Lockington D, Volker R (1999b) Truncation errors in finite difference models for solute transport equation with first-order reaction. J Contam Hydrol 35:409–428

Ataie-Ashtiani B, Hosseini S (2005a) Error analysis of finite difference methods for two-dimensional advection–dispersion–reaction equation. Adv Water Resour 28:793–806

Ataie-Ashtiani B, Hosseini S (2005b) Numerical errors of explicit finite difference approximation for two-dimensional solute transport equation with linear sorption. Environ Modell Softw 20:817–826

Bear J (1972) Dynamics of fluids in porous media. Elsevier Science, New York

Bresler E (1973) Simultaneous transport of solutes and water under transient unsaturated flow conditions. Water Resour Res 9:975–986

Campbell JE, Longsine DE, Reeves M (1981) Distributed velocity method of solving the convective-dispersion equation: 1. introduction, mathematical theory, and numerical implementation. Adv Water Resour 4:102–108

Chaudhari NM (1971) An improved numerical technique for solving multidimensional miscible displacement equations. Soc Petrol Eng J 11:277–284

De Smedt F, Wierenga P (1977) Simulation of water and solute transport in unsaturated soils. In: Proceedings of 3rd international symposium in hydrology. Fort Collins

Dudley L, McLean J, Furst T, Jurinak J (1991) Sorption of cadmium and copper from an acid mine waste extract by two calcareous soils: Column studies. Soil Sci 151:2

Ferziger JH, Perić M (1999) Computational methods for fluid dynamics. Springer, New York

Gresho P, Sani R (1998) Incompressible flow and the finite element method: advection-diffusion and isothermal laminar flow, vol 1. Wiley, New York

Igboekwe MU, Gurunadha Rao VVS, Ok-wueze EE (2008) Groundwater flow modelling of Kwa Ibo River watershed Southeastern Nigeria. Hydrol Process 22:1523–1531

Lantz R (1971) Quantitative evaluation of numerical diffusion (truncation error). Soc Petrol Eng J 11:315–320

May R, Noye BJ (1984) The numerical solution of ordinary differential equations: initial value problems. In: Noye B (ed) Computational techniques for differential equations. North-Holland, NewYork

Moldrup P, Yamaguchi T, Hansen J, Rolston D (1992) An accurate and numerically stable model for one-dimensional solute transport in soils. Soil Sci 153:261–273

Moldrup P, Yamaguchi T, Ralston EVK, Hansen J (1994a) Removing numerically induced dispersion from finite difference models for solute and water transport in unsaturated soils. Soil Sci 157:153–161

Moldrup P, Paulsen T, Rolston D, Yamaguchi T, Hansen J (1994b) Integrated flux model for unsteady transport of trace organic chemicals in soils. Soil Sci 157:137–152

Notodarmojo S, Ho G, Scott W, Davis G (1991) Modelling phosphorus transport in soils and groundwater with two-consecutive reactions. Water Res 25:1205–1216

Noye BJ, Hayman K (1985) Accurate finite difference methods for solving the advection-diffusion equation. In: Noye B, May R (eds) Computational techniques and applications: CTAC-85. North-Holland, NewYork, pp 137–157

Noye BJ (1978) Finite difference techniques. In: Noye B (ed) Numerical simulation of fluid motion. North-Holland, NewYork, pp 1–112

Noye BJ (1990) A new third-order finite-difference method for transient one-dimensional advection–diffusion. Commun Appl Numer M 6:279–288

Pinder GF, Gray WG (1977) Finite element simulation in surface and subsurface hydrology. Academic Press, New York

Sheu TW, Wang S, Lin R (2000) An implicit scheme for solving the convection–diffusion–reaction equation in two dimensions. J Comput Phys 164:123–142

Simmons CT, Narayan KA, Wooding RA (1999) On a test case for density-dependent groundwater flow and solute transport models: the salt lake problem. Water Resour Res 35:3607–3620

Van Genuchten MTh, Wierenga PJ (1974) Simulation of one-dimensional solute transfer in porous media. AES Bull, New Mexico State University, Las Cruces, New Mexico, p 628

Van Genuchten MTh, Gray WG (1978) Analysis of some dispersion corrected numerical schemes for solution of the transport equation. Int J Numer Meth Eng 12:387–404

Van Genuchten MT, Alves W (1982) Analytical solutions of the one dimensional convective-dispersive solute transport equation. Technical Bulletin, No. 1661, US. Department of Agriculture, p 155

Woods J, Simmons CT, Narayan KA, Tuck E, Stott J (eds) (1998) Verification of black box groundwater models. In: Third biennial engineering mathematics and applications conference: EMAC98, Australia, pp 523–526

Woods JM, Teubner D, Simmons CT, Narayan KA (1999) Numerical inaccuracy in groundwater modelling: diagnosis and pathology. In: Joint congress of the 25th hydrology and water resources symposium and the 2nd international conference on water resources and environmental research "Water 99", Australia

Zheng C (1999) MT3D: a modular three-dimensional transport model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems. Report to U.S. Environmental Protection Agency, Ada, OK, p 170