Journal of Contaminant Hydrology 35 (1999) 409–428

JOURNAL OF Contaminant Hydrology

Truncation errors in finite difference models for solute transport equation with first-order reaction

B. Ataie-Ashtiani [a], D.A. Lockington [b,*], R.E. Volker [b]

[a] *Department of Civil Engineering, Sharif University of Technology, Tehran, Iran*

[b] *Department of Civil Engineering, University of Queensland, Brisbane, Queensland 4072, Australia*

Received 2 December 1997; accepted 13 July 1998

Abstract

The truncation errors associated with finite difference solutions of the advection-dispersion equation with first-order reaction are formulated from a Taylor analysis. The error expressions are based on a general form of the corresponding difference equation and a temporally and spatially weighted parametric approach is used for differentiating among the various finite difference schemes. The numerical truncation errors are defined using Peclet and Courant numbers and a new Sink/Source dimensionless number. It is shown that all of the finite difference schemes suffer from truncation errors. In particular it is shown that the Crank–Nicolson approximation scheme does not have second order accuracy for this case. The effects of these truncation errors on the solution of an advection–dispersion equation with a first order reaction term are demonstrated by comparison with an analytical solution. The results show that these errors are not negligible and that correcting the finite difference scheme for them results in a more accurate solution.

Keywords: Advection–dispersion equation; Finite difference model; Truncation error; First-order reaction

1. Introduction

Approximating differential equations in finite difference (FD) models by discretization introduces truncation errors. In the case of transport equations like the advection–

* Corresponding author. University of Queensland, Dep. of Civil Engineering, St. Lucia Qld 4067, Australia. E-mail: d.lockington@mailbox.uq.edu.au

PII: S0169-7722(98)00106-5

dispersion equation (ADE), numerical dispersion is a well-known consequence of truncation error. Numerical dispersion was first quantified by Lantz (1971), and Chaudhari (1971) as a second-order error term through examination of the truncated Taylor series approximation of a simple, explicit FD solution of the basic, one-dimensional ADE. Although for the case of this ADE the numerical dispersion is the only truncation error, for the more general transport equation (e.g., with reaction) other truncation errors are introduced.

Typically, numerical studies consider the effect of numerical dispersion (e.g., De Smedt and Wierenga, 1977; van Genuchten and Gray, 1978; Notodarmojo et al., 1991; Dudley et al., 1991; Moldrup et al., 1992, 1994a,b). The zero- and first-order truncation errors in the ADE with reaction (ADER) were quantified for the first time by Ataie-Ashtiani et al. (1995a). Also Ataie-Ashtiani et al. (1995b) showed that in some FD schemes the variable spatial discretization caused a first order truncation error in the FD solution of the conventional ADE. Ataie-Ashtiani et al. (1996) proposed the correction method for the numerical truncation errors of an explicit centred in space scheme. Moldrup et al. (1996) applied the same idea for correcting an explicit FD approximation of the one-dimensional diffusion–reaction equation. In their work, they include the effects of third and higher order temporal derivatives.

The primary objectives of this paper are to derive the analytical expressions for truncation errors for the general FD form of the ADER that covers explicit, Crank–Nicolson, and implicit schemes and to show that none of the widely used FD schemes have second order accuracy for solving the ADER. In fact, all of these schemes do not have even zeroth order accuracy. Finally, the effect of the correction of these truncation errors are discussed.

2. One-dimensional ADER

The partial differential equation describing one-dimensional transient transport of solutes through a homogeneous soil, including first-order reaction or a concentration-dependent sink/source is written as

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - u\frac{\partial C}{\partial z} - kC \tag{1}$$

where C is solute concentration (M L^{-3}), t is time (T), z is vertical distance (L), u is the discharge per unit area (L T^{-1}), D is the dispersion coefficient (L^2 T^{-1}), and k is the first-order reaction rate coefficient (T^{-1}).

It should be noted that the transport parameters are considered constants only within each combination of time and depth increments in the calculations; otherwise the parameters are considered variable.

3. Finite difference approximation of ADER

The general form of FD approximation of Eq. (2), using ω and α as the temporal weighting and spatial weighting parameters, may be expressed as

$$\frac{C_i^{n+1}-C_i^n}{\Delta t} = D\left[\omega\frac{C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}}{\Delta z^2}+(1-\omega)\frac{C_{i+1}^n-2C_i^n+C_{i-1}^n}{\Delta z^2}\right]$$
$$-u\left[\omega\frac{(1-\alpha)C_i^{n+1}+\alpha C_{i+1}^{n+1}-(1-\alpha)C_{i-1}^{n+1}-\alpha C_i^{n+1}}{\Delta z}\right.$$
$$\left.+(1-\omega)\frac{(1-\alpha)C_i^n+\alpha C_{i+1}^n-(1-\alpha)C_{i-1}^n-\alpha C_i^n}{\Delta z}\right]$$
$$-k\left[\omega C_i^{n+1}+(1-\omega)C_i^n\right] \quad (2)$$

where the superscript n refers to time, the subscript i refers to depth, Δt is the time increment (T) and Δz is the depth increment (L) used in the calculations.

The FD scheme reduces to the backward in time or implicit scheme when ω is 1, to the centred in time or Crank–Nicolson scheme when ω is 0.5, and to forward in time or explicit scheme when ω is 0. The value of α determines the type of spatial discretization, and the most obvious choice of α is 0.5, which is referred to as the centred in distance scheme. An alternative spatial weighting scheme is the upstream or upwind scheme, which is defined by α equals 0 if $u > 0$ and α equals 1 if $u < 0$.

A Taylor series expansion of C about any grid point is used to determine the form of the truncation errors (Lantz, 1971; Chaudhari, 1971; Moldrup et al., 1994b). If the third and higher order spatial derivatives are neglected, as they are not present in the original transport equation, then

$$C_{i+1}^n \approx C_i^n + \Delta z\frac{\partial C}{\partial z}+\frac{\Delta z^2}{2}\frac{\partial^2 C}{\partial z^2} \quad (3)$$

$$C_{i-1}^n = C_i^n - \Delta z\frac{\partial C}{\partial z}+\frac{\Delta z^2}{2}\frac{\partial^2 C}{\partial z^2} \quad (4)$$

$$C_i^{n+1} \approx C_i^n + \sum_{m=1}^{\infty}\left(\frac{\Delta t^m}{m!}\frac{\partial^m C}{\partial t^m}\right) \quad (5)$$

$$C_{i+1}^{n+1} \approx C_i^{n+1} + \Delta z\frac{\partial C^{n+1}}{\partial z}+\frac{\Delta z^2}{2}\frac{\partial^2 C^{n+1}}{\partial z^2} \quad (6)$$

$$C_{i-1}^{n+1} = C_i^{n+1} - \Delta z\frac{\partial C^{n+1}}{\partial z}+\frac{\Delta z^2}{2}\frac{\partial^2 C^{n+1}}{\partial z^2} \quad (7)$$

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), again the third and higher order spatial derivatives are neglected. It is noticed that the transport parameters are assumed constant within each combination of time and depth increments in the finite difference calculations. Thus

$$\frac{\partial^2 C}{\partial t^2} = D\frac{\partial^2}{\partial z^2}\left(\frac{\partial C}{\partial t}\right) - u\frac{\partial}{\partial z}\left(\frac{\partial C}{\partial t}\right) - k\left(\frac{\partial C}{\partial t}\right) \approx (u^2 - 2kD)\frac{\partial^2 C}{\partial z^2} + 2ku\frac{\partial C}{\partial z} + k^2 C \tag{8}$$

Analogously,

$$\frac{\partial^3 C}{\partial t^3} \approx (-3ku^2 + 3k^2 D)\frac{\partial^2 C}{\partial z^2} - 3k^2 u\frac{\partial C}{\partial z} - k^3 C \tag{9}$$

$$\frac{\partial^4 C}{\partial t^4} \approx (6k^2u^2 - 4k^3 D)\frac{\partial^2 C}{\partial z^2} + 4k^3 u\frac{\partial C}{\partial z} + k^4 C \tag{10}$$

or in general, for $m \geq 2$

$$\frac{\partial^m C}{\partial t^m} \approx (-1)^m\left(\frac{m(m-1)}{2}k^{m-2}u^2 - mk^{m-1}D\right)\frac{\partial^2 C}{\partial z^2} + (-1)^m mk^{m-1}u\frac{\partial C}{\partial z} + (-1)^m k^m C \tag{11}$$

Therefore, Eq. (5) is written as

$$C_i^{n+1} \approx C_i^n + \Delta t\frac{\partial C}{\partial t} + \sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m\left(\frac{m(m-1)}{2}k^{m-2}u^2 - mk^{m-1}D\right)\frac{\partial^2 C}{\partial z^2} + (-1)^m mk^{m-1}u\frac{\partial C}{\partial z} + (-1)^m k^m C\right] \tag{12}$$

Inserting Eq. (12) in Eqs. (6) and (7) and neglecting the spatial derivatives of third and higher order, and considering

$$\frac{\partial^2 C}{\partial z \partial t} = D\frac{\partial^3 C}{\partial z^3} - u\frac{\partial^2 C}{\partial z^2} - k\frac{\partial C}{\partial z} \tag{13}$$

$$\frac{\partial^3 C}{\partial z^2 \partial t} = D\frac{\partial^4 C}{\partial z^4} - u\frac{\partial^3 C}{\partial z^3} - k\frac{\partial^2 C}{\partial z^2} \tag{14}$$

yields

$$\begin{aligned} C_{i+1}^{n+1} \approx{} & C_i^n + \Delta t\frac{\partial C}{\partial t} + \sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m\left(\frac{m(m-1)}{2}k^{m-2}u^2 - mk^{m-1}D\right)\frac{\partial^2 C}{\partial z^2}\right. \\ & \left. + (-1)^m mk^{m-1}u\frac{\partial C}{\partial z} + (-1)^m k^m C\right] + \Delta z\frac{\partial C}{\partial z} + \Delta t\Delta z\left(-u\frac{\partial^2 C}{\partial z^2}\right. \\ & \left. - k\frac{\partial C}{\partial z}\right) + \Delta z\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m mk^{m-1}u\frac{\partial^2 C}{\partial z^2} + (-1)^m k^m\frac{\partial C}{\partial z}\right] \\ & + \frac{\Delta z^2}{2}\frac{\partial^2 C}{\partial z^2} - \frac{\Delta z^2 \Delta t}{2}k\frac{\partial^2 C}{\partial z^2}z + \frac{\Delta z^2}{2}\sum_{m=2}^{\infty}\frac{\Delta t^m}{m!}\left[(-1)^m k^m\frac{\partial^2 C}{\partial z^2}\right] \end{aligned} \tag{15}$$

$$C_{i-1}^{n+1} \approx C_i^n + \Delta t \frac{\partial C}{\partial t} + \sum_{m=2}^{\infty} \frac{\Delta t^m}{m!} \left[(-1)^m \left(\frac{m(m-1)}{2} k^{m-2} u^2 - mk^{m-1} D \right) \frac{\partial^2 C}{\partial z^2} \right.$$
$$\left. + (-1)^m mk^{m-1} u \frac{\partial C}{\partial z} + (-1)^m k^m C \right] - \Delta z \frac{\partial C}{\partial z} - \Delta t \Delta z \left(-u \frac{\partial^2 C}{\partial z^2} \right.$$
$$\left. - k \frac{\partial C}{\partial z} \right) - \Delta z \sum_{m=2}^{\infty} \frac{\Delta t^m}{m!} \left[(-1)^m mk^{m-1} u \frac{\partial^2 C}{\partial z^2} + (-1)^m k^m \frac{\partial C}{\partial z} \right]$$
$$+ \frac{\Delta z^2}{2} \frac{\partial^2 C}{\partial z^2} - \frac{\Delta z^2 \Delta t}{2} k \frac{\partial^2 C}{\partial z^2} + \frac{\Delta z^2}{2} \sum_{m=2}^{\infty} \frac{\Delta t^m}{m!} \left[(-1)^m k^m \frac{\partial^2 C}{\partial z^2} \right] \quad (16)$$

Substituting Eqs. (3)–(5), (15) and (16) in Eq. (2) gives

$$\frac{\partial C}{\partial t} = \left\{ D - 2\omega \Delta t k D + \left(\alpha - \frac{1}{2} \right) \omega \Delta z \Delta t u k + \left(\frac{1}{2} - \alpha \right) \Delta z u + \omega \Delta t u^2 \right.$$
$$+ \sum_{m=2}^{\infty} \left[\frac{\Delta t^{m-1}}{(m-1)!} (-1)^m \left(\frac{m-1}{2} k^{m-2} u^2 - k^{m-1} D \right) \right] (-1 - \omega k \Delta t)$$
$$+ \sum_{m=2}^{\infty} \left[\frac{\Delta t^m}{(m-1)!} (-1)^m k^{m-1} u \right] (-\omega u) + \sum_{m=2}^{\infty} \left[\frac{\Delta t^m}{m!} (-1)^m k^m \right]$$
$$\left. \times \left(\omega D - \omega \alpha u \Delta z + \omega \frac{\Delta z u}{2} \right) \right\} \frac{\partial^2 C}{\partial z^2} - \left\{ u - 2\omega \Delta t k u \right.$$
$$+ \sum_{m=2}^{\infty} \left[\frac{\Delta t^{m-1}}{(m-1)!} (-1)^m k^{m-1} u \right] (1 + \omega k \Delta t)$$
$$\left. + \sum_{m=2}^{\infty} \left[\frac{\Delta t^m}{m!} (-1)^m k^m \right] \omega u \right\} \frac{\partial C}{\partial z} - \left\{ k - \omega \Delta t k^2 \right.$$
$$\left. + \sum_{m=2}^{\infty} \left[\frac{\Delta t^{m-1}}{m!} (-1)^m k^m \right] (1 + \omega \Delta t k) \right\} C \quad (17)$$

4. Truncation error formulations

A comparison between Eq. (17) and the original governing differential equation shows that the discretization introduces three forms of truncation error. They can be identified as a second-order truncation error or numerical dispersion, D_{num}

$$D_{\mathrm{num}} = \left\{ -2\omega\Delta tkD + \left(\alpha - \frac{1}{2}\right)\omega\Delta z\Delta tuk + \left(\frac{1}{2} - \alpha\right)\Delta zu + \omega\Delta tu^2 + \sum_{m=2}^{\infty}\left[\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m\left(\frac{m-1}{2}k^{m-2}u^2 - k^{m-1}D\right)\right](-1-\omega k\Delta t) + \sum_{m=2}^{\infty}\left[\frac{\Delta t^m}{(m-1)!}(-1)^m k^{m-1}u\right](-\omega u) + \sum_{m=2}^{\infty}\left[\frac{\Delta t^m}{m!}(-1)^m k^m\right] \times \left(\omega D - \omega\alpha u\Delta z + \omega\frac{\Delta zu}{2}\right)\right\} \tag{18}$$

a first-order truncation error or numerical water velocity, u_{num}

$$u_{\mathrm{num}} = \left\{ -2\omega\Delta tku + \sum_{m=2}^{\infty}\left[\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m k^{m-1}u\right](1+\omega k\Delta t) + \sum_{m=2}^{\infty}\left[\frac{\Delta t^m}{m!}(-1)^m k^m\right]\omega u\right\} \tag{19}$$

and a zero-order truncation error or numerical reaction coefficient, k_{num}

$$k_{\mathrm{num}} = -\omega\Delta tk^2 + \sum_{m=2}^{\infty}\left[\frac{\Delta t^{m-1}}{m!}(-1)^m k^m\right](1+\omega\Delta tk) \tag{20}$$

Using the Peclet number, Pe, Courant number, Cr, and introducing a Sink/Source number, Sr, as follows;

$$\mathrm{Pe} = \frac{u\Delta z}{D} \tag{21}$$

$$\mathrm{Cr} = \frac{u\Delta t}{\Delta z} \tag{22}$$

$$\mathrm{Sr} = k\Delta t \tag{23}$$

Eqs. (18)–(20) can be expressed as a function of the dimensionless numbers, Pe, Cr, and Sr,

$$\frac{D_{\mathrm{num}}}{D} = \left\{ -2\omega\mathrm{Sr} + \left(\alpha - \frac{1}{2}\right)\omega\mathrm{SrPe} + \left(\frac{1}{2} - \alpha\right)\mathrm{Pe} + \omega\mathrm{PeCr} - \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\left(\frac{m-1}{2}\mathrm{Sr}^{m-2}\mathrm{PeCr} - \mathrm{Sr}^{m-1}\right)\right](1+\omega\mathrm{Sr}) - \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\omega\mathrm{Sr}^{m-1}\mathrm{PeCr}\right] + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\mathrm{Sr}^m\right] \times \left(\omega - \omega\alpha\mathrm{Pe} + \omega\frac{\mathrm{Pe}}{2}\right)\right\} \tag{24}$$

$$\frac{u_{\mathrm{num}}}{u} = \left\{ -2\omega \mathrm{Sr} + \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} \mathrm{Sr}^{m-1} \right] (1+\omega \mathrm{Sr}) + \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{m!} \mathrm{Sr}^{m} \right] \omega \right\} \tag{25}$$

$$\frac{k_{\mathrm{num}}}{k} = -\omega \mathrm{Sr} + \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{m!} \mathrm{Sr}^{m-1} \right] (1+\omega Sr) \tag{26}$$

The ratio of truncation terms to the corresponding physical terms for different FD schemes are as follows:(1) Explicit approximation, upstream weighting with positive velocity ($\omega = 0,\ \alpha = 0$ with $u > 0$):

$$\frac{D_{\mathrm{num}}}{D} = \frac{\mathrm{Pe}}{2} - \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} \left(\frac{m-1}{2} \mathrm{Sr}^{m-2} \mathrm{PeCr} - \mathrm{Sr}^{m-1} \right) \right] \tag{27}$$

$$\frac{u_{\mathrm{num}}}{u} = \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} Sr^{m-1} \right] \tag{28}$$

$$\frac{k_{\mathrm{num}}}{k} = \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{m!} \mathrm{Sr}^{m-1} \right] \tag{29}$$

(2) Explicit approximation, centred in distance ($\omega = 0,\ \alpha = 0.5$):

$$\frac{D_{\mathrm{num}}}{D} = -\sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} \left(\frac{m-1}{2} \mathrm{Sr}^{m-2} \mathrm{PeCr} - \mathrm{Sr}^{m-1} \right) \right] \tag{30}$$

$$\frac{u_{\mathrm{num}}}{u} = \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} \mathrm{Sr}^{m-1} \right] \tag{31}$$

$$\frac{k_{\mathrm{num}}}{k} = \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{m!} \mathrm{Sr}^{m-1} \right] \tag{32}$$

(3) Crank–Nicolson approximation, upstream weighting with positive velocity ($\omega = 0.5$, $\alpha = 0$ with $u > 0$):

$$\begin{aligned} \frac{D_{\mathrm{num}}}{D} = \Bigg\{ & -\mathrm{Sr} - \frac{\mathrm{SrPe}}{4} + \frac{\mathrm{Pe}}{2} + \frac{\mathrm{PeCr}}{2} \\ & - \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} \left(\frac{m-1}{2} \mathrm{Sr}^{m-2} \mathrm{PeCr} - \mathrm{Sr}^{m-1} \right) \right] \left(1 + \frac{Sr}{2} \right) \\ & - \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} \frac{\mathrm{Sr}^{m-1} \mathrm{PeCr}}{2} \right] + \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{m!} \mathrm{Sr}^{m} \right] \left(\frac{1}{2} + \frac{\mathrm{Pe}}{4} \right) \Bigg\} \end{aligned} \tag{33}$$

$$\frac{u_{\mathrm{num}}}{u} = -\mathrm{Sr} + \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{(m-1)!} \mathrm{Sr}^{m-1} \right] \left(1 + \frac{\mathrm{Sr}}{2} \right) + \sum_{m=2}^{\infty} \left[\frac{(-1)^m}{m!} \frac{\mathrm{Sr}^{m}}{2} \right] \tag{34}$$

$$\frac{k_{\text{num}}}{k} = -\frac{\text{Sr}}{2} + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}Sr^{m-1}\right]\left(1+\frac{\text{Sr}}{2}\right) \tag{35}$$

(4) Crank–Nicolson approximation, centred in distance ($\omega = 0.5$, $\alpha = 0.5$):

$$\frac{D_{\text{num}}}{D} = \left\{-\text{Sr} + \frac{\text{PeCr}}{2} - \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\left(\frac{m-1}{2}\text{Sr}^{m-2}\text{PeCr} - \text{Sr}^{m-1}\right)\right]\right.$$
$$\left.\times\left(1+\frac{\text{Sr}}{2}\right) - \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\frac{Sr^{m-1}\text{PeCr}}{2}\right] + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\frac{\text{Sr}^m}{2}\right]\right\} \tag{36}$$

$$\frac{u_{\text{num}}}{u} = -\text{Sr} + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\text{Sr}^{m-1}\right]\left(1+\frac{\text{Sr}}{2}\right) + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\frac{\text{Sr}^m}{2}\right] \tag{37}$$

$$\frac{k_{\text{num}}}{k} = -\frac{\text{Sr}}{2} + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\text{Sr}^{m-1}\right]\left(1+\frac{\text{Sr}}{2}\right) \tag{38}$$

(5) Implicit approximation, upstream weighting with positive velocity ($\omega = 1$, $\alpha = 0$ with $u > 0$):

$$\frac{D_{\text{num}}}{D} = \left\{-2\text{Sr} - \frac{\text{SrPe}}{2} + \frac{\text{Pe}}{2} + \text{PeCr}\right.$$
$$- \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\left(\frac{m-1}{2}\text{Sr}^{m-2}\text{PeCr} - \text{Sr}^{m-1}\right)\right](1+\text{Sr})$$
$$\left.- \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\text{Sr}^{m-1}\text{PeCr}\right] + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\text{Sr}^m\right]\left(1+\frac{\text{Pe}}{2}\right)\right\} \tag{39}$$

$$\frac{u_{\text{num}}}{u} = -2\text{Sr} + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\text{Sr}^{m-1}\right](1+\text{Sr}) + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\text{Sr}^m\right] \tag{40}$$

$$\frac{k_{\text{num}}}{k} = -\text{Sr} + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\text{Sr}^{m-1}\right](1+\text{Sr}) \tag{41}$$

(6) Implicit approximation, centred in distance ($\omega = 1$, $\alpha = 0.5$):

$$\frac{D_{\text{num}}}{D} = \left\{-2\text{Sr} + \text{PeCr} - \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\left(\frac{m-1}{2}\text{Sr}^{m-2}\text{PeCr} - \text{Sr}^{m-1}\right)\right]\right.$$
$$\left.\times(1+\text{Sr}) - \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\text{Sr}^{m-1}\text{PeCr}\right] + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\text{Sr}^m\right]\right\} \tag{42}$$

$$\frac{u_{\text{num}}}{u} = -2\text{Sr} + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{(m-1)!}\text{Sr}^{m-1}\right](1+\text{Sr}) + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\text{Sr}^{m}\right] \tag{43}$$

$$\frac{k_{\text{num}}}{k} = -\text{Sr} + \sum_{m=2}^{\infty}\left[\frac{(-1)^m}{m!}\text{Sr}^{m-1}\right](1+\text{Sr}) \tag{44}$$

As seen, none of these methods is free of truncation errors and the widely used assumption of zero numerical dispersion in Crank–Nicolson with a centred-in-distance approximation is not valid for the ADER. The zeroth and first order truncation errors for all schemes are functions of Sr only and therefore are zero for the conventional ADE when k is zero.

Eqs. (27)–(44) present D_{num}/D, u_{num}/u and k_{num}/k as infinite series. Figs. 1–3 show the convergence of these parameters for explicit-, Crank–Nicolson- and implicit-upstream approximation in an example case when Pe = 1 and Cr = 1. For Sr less than 0.2 just two components ($m = 3$) of the series gives a very good approximation of truncation errors. Including a maximum of four terms ($m = 5$) of the series gives enough accuracy in the calculation of truncation errors for the higher values of Sr. Also based on these figures, it can be concluded that the absolute values of u_{num}/u and k_{num}/k increase for all schemes with increasing Sink/Source number, Sr.

The ratio of numerical to physical dispersion coefficient, considering three terms of the series ($m = 4$), as a function of Pe and Cr for two different values of Sr, 0.1 and 0.8, is illustrated in Figs. 4–6 for explicit, Crank–Nicolson, and implicit discretization schemes, respectively. The figures demonstrate that for the small value of Sr, numerical dispersion increases with increasing Pe and Cr in general, except for the Crank–Nicolson upstream scheme where increasing the Courant number leads to a decrease in numerical dispersion. However, this trend is not observed for larger Sr. No trend is seen between Sr and numerical dispersion (ie; numerical dispersion increases in some cases and decreases in others with increasing Sr).

Fig. 5 shows that for small values of Sr the Crank–Nicolson centred-in-distance approximation has the smallest numerical dispersion in comparison with the other schemes, but this is not the case when Sr increases. In conclusion, Figs. 4–6 show that the accuracy of the numerical approximation for the ADER not only depends on Pe and Cr, as the conventional ADE does, but also on the value of Sr.

5. Removing truncation errors

The effect of zero, first and second order truncation errors on the results of the explicit and Crank–Nicolson FD schemes which are the most widely used FD schemes, is illustrated here. The Crank–Nicolson scheme is well-known because of its accuracy and stability while the advantage of the explicit scheme is its simplicity. Although it is subject to a stability criterion, the explicit scheme has been implemented in a number of commonly used transport simulation models, i.e., the MOC code by Konikow and Bredehoeft (1978) and the MT3D code by Zheng (1990).

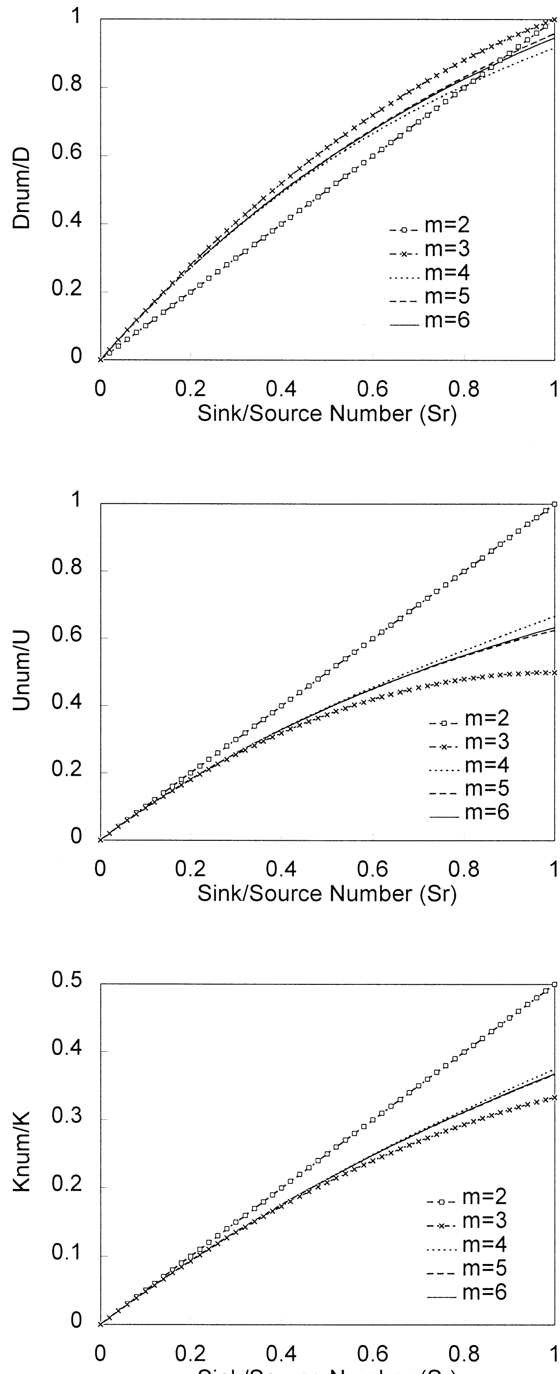


Fig. 1. D_{num}/D, u_{num}/u and k_{num}/k convergence for explicit–upstream scheme when Pe = 1 and Cr = 1.

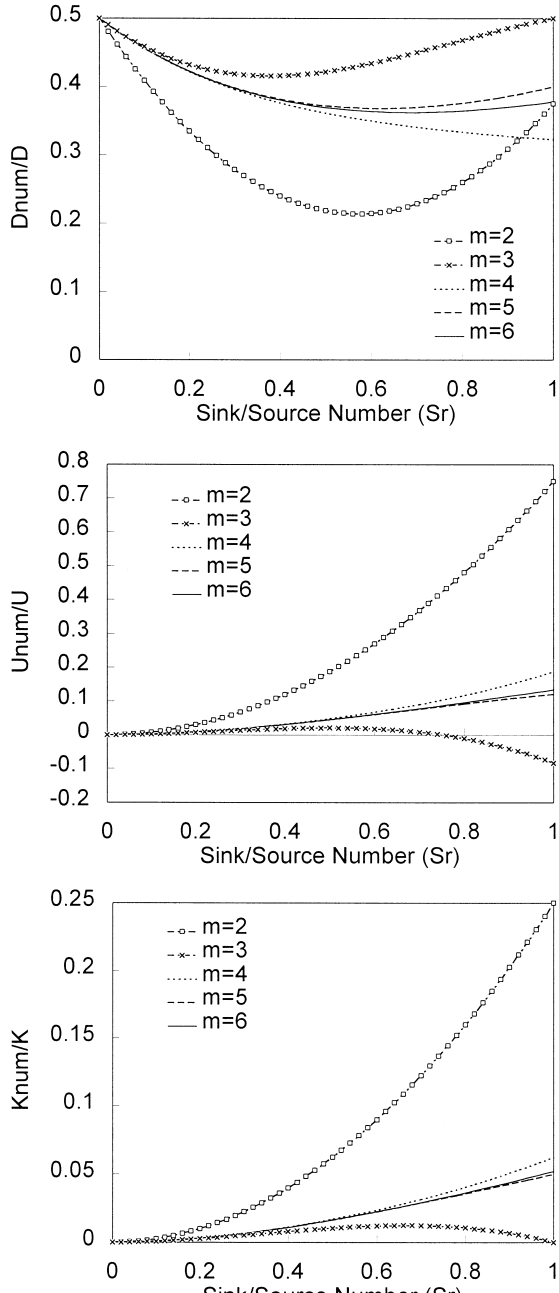


Fig. 2. D_{num} / D, u_{num} / u and k_{num} / k convergence for Crank–Nicolson–upstream scheme when Pe = 1 and Cr = 1.

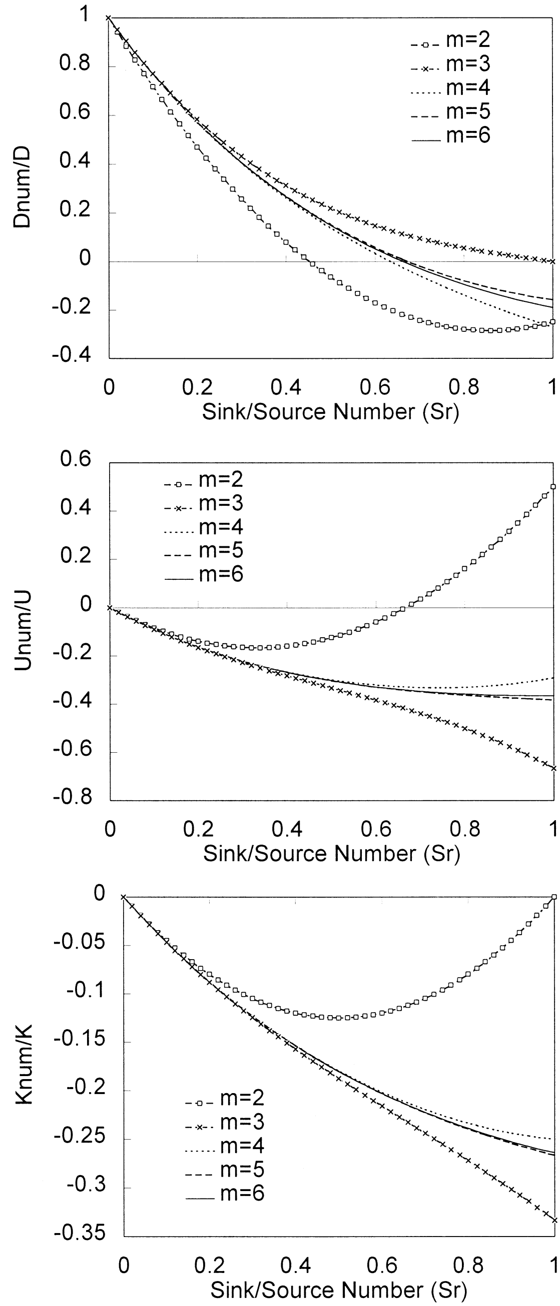


Fig. 3. D_{num}/D, u_{num}/u and k_{num}/k convergence for implicit–upstream scheme when Pe = 1 and Cr = 1. (a) explicit, upstream for Sr = 0.1. (b) explicit, upstream for Sr = 0.8. (c) explicit, centred for Sr = 0.1. (d) explicit, centred for Sr = 0.8.

To remove the induced numerical truncation errors from the general finite difference model, Eq. (2) is rewritten as:

$$\frac{C_i^{n+1}-C_i^n}{\Delta t} = D*\left[\omega\frac{C_{i+1}^{n+1}-2C_i^{n+1}+C_{i-1}^{n+1}}{\Delta z^2}+(1-\omega)\frac{C_{i+1}^{n}-2C_i^{n}+C_{i-1}^{n}}{\Delta z^2}\right]$$
$$-u*\left[\omega\frac{(1-\alpha)C_i^{n+1}-\alpha C_{i+1}^{n+1}-(1-\alpha)C_{i-1}^{n+1}-\alpha C_i^{n+1}}{\Delta z}\right.$$
$$\left.+(1-\omega)\frac{(1-\alpha)C_i^{n}+\alpha C_{i+1}^{n}-(1-\alpha)C_{i-1}^{n}-\alpha C_i^{n}}{\Delta z}\right]$$
$$-k*\left[\omega C_i^{n+1}+(1-\omega)C_i^n\right]$$
$$where\, D{=\!=}D-D_{num}, u*=u-u_{num}, k*=k-k_{num}. \tag{45}$$

where $D*=D-D_{\text{num}}$, $u*=u-u_{\text{num}}$, $k*=k-k_{\text{num}}$.

The effect of zero, first and second order truncation errors on the results of the explicit and Crank–Nicolson FD schemes is assessed by comparing the FD model results with the van Genuchten and Alves (1982) analytical solution. According to van Genuchten and Alves (1982), in the case of constant u, D, and k, the analytical solution for Eq. (1) for the initial and boundary conditions

$$\begin{array}{lll} C=0 & t=0 & z>0 \\ C=C_0 & t>0 & z=0 \\ C=0 & t>0 & z\to\infty \end{array}$$

is

$$C(z,t)=\frac{C_0}{2}\exp\left[\left[\frac{(u-\upsilon)z}{2D}\right]\text{erfc}\left[\frac{z-\upsilon t}{2(Dt)^{\frac{1}{2}}}\right]\right.$$
$$\left.+\exp\left[\frac{(u+\upsilon)z}{2D}\right]\text{erfc}\left[\frac{z+\upsilon t}{2(Dt)^{\frac{1}{2}}}\right]\right] \tag{46}$$

where

$$\upsilon=(u^2+4kD)^{0.5}$$

A semi-infinite column is considered with the parameter values $u=5$ mm h^{-1}, $D=100$ mm^2 h^{-1}, $k=0.1$ h^{-1}, and C_0 is taken as 1000.0 mg l^{-1}. This problem is solved with $\Delta z=20$ mm and $\Delta t=1.0$ h. Therefore, the dimensionless numbers, Pe, Cr, and Sr for this case are 1, 0.25, and 0.1, respectively.

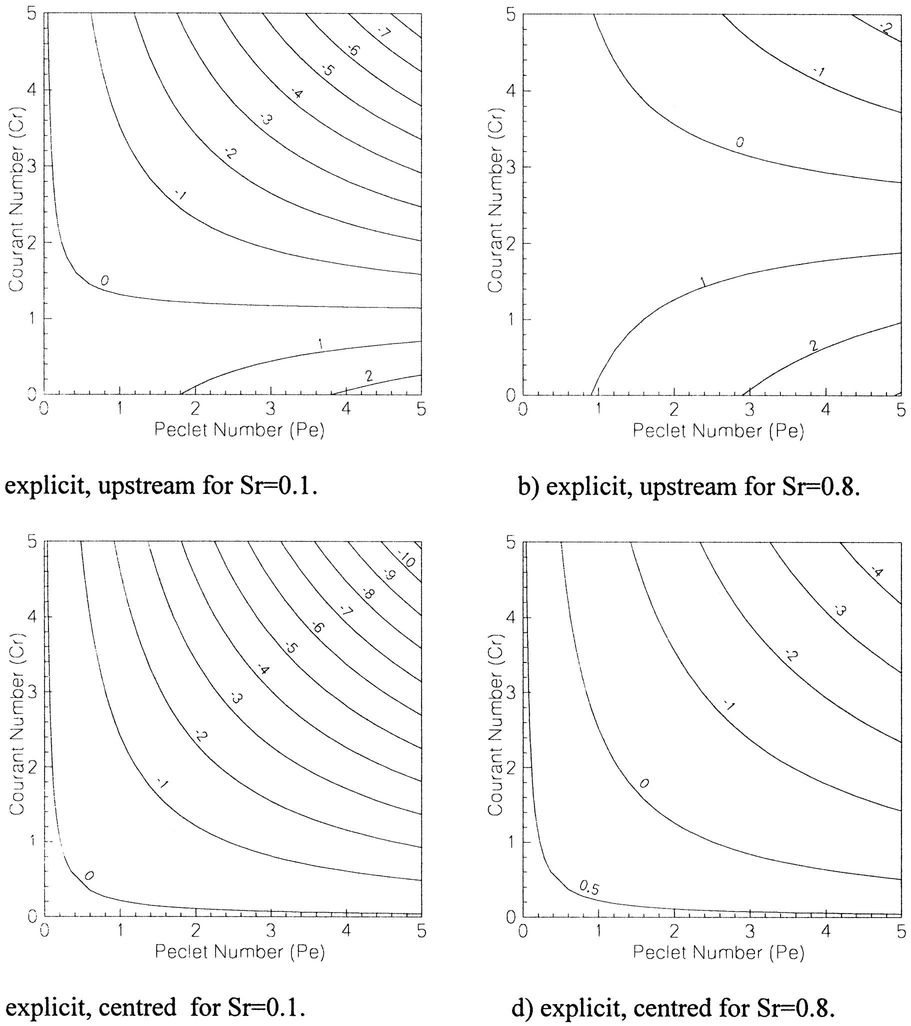
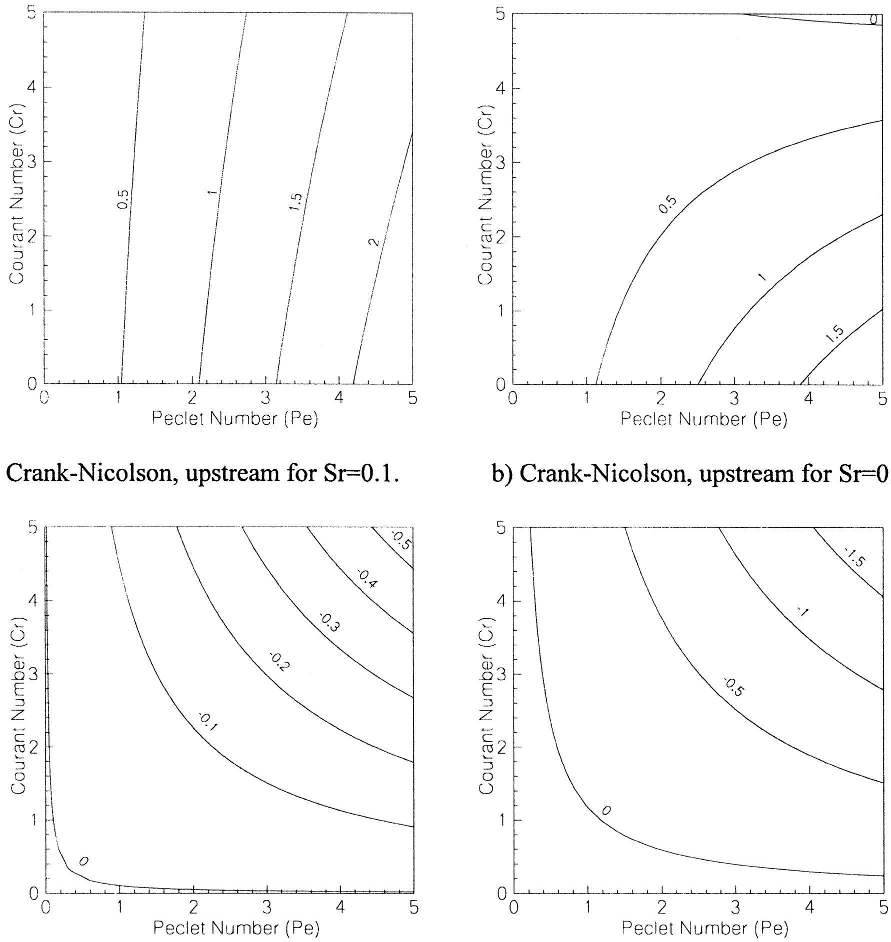


Fig. 4. Ratio of numerical dispersion coefficient to physical dispersion coefficient for explicit schemes. (a) Crank–Nicolson, upstream for Sr = 0.1. (b) Crank–Nicolson, upstream for Sr = 0.8. (c) Crank–Nicolson, centred for Sr = 0.1. (d) Crank–Nicolson, centred for Sr = 0.8.

The stability criteria of the explicit centred in space scheme for ADER was determined by Ataie-Ashtiani et al. (1996), using the matrix method proposed by Smith (1978), as follows:

$$\Delta t \leq \frac{1}{\dfrac{2D*}{\Delta z^2} + \dfrac{k*}{2}} \tag{47}$$

$$\Delta t \leq \frac{\Delta z}{u*} \tag{48}$$



a) Crank-Nicolson, upstream for Sr=0.1.

b) Crank-Nicolson, upstream for Sr=0.8.

c) Crank-Nicolson, centred for Sr=0.1.

d) Crank-Nicolson, centred for Sr=0.8.

Fig. 5. Ratio of numerical dispersion coefficient to physical dispersion coefficient for Crank–Nicolson schemes. (a) Implicit, upstream for $Sr = 0.1$. (b) Implicit, upstream for $Sr = 0.8$. (c) Implicit, centred for $Sr = 0.1$. (d) Implicit, centred for $Sr = 0.8$.

If the same method is applied for the explicit upstream scheme, the result is

$$\Delta t \le \frac{1}{\dfrac{2D*}{\Delta z^2} + \dfrac{u*}{\Delta z} + \dfrac{k*}{2}} \tag{49}$$

Fig. 7 shows the concentration ratio, C/C_0, against depth for the analytical solution and numerical solution in the cases without correction and with correction for truncation errors. Fig. 7 shows that the correction of truncation errors is very effective in improving the results of the explicit upstream FD scheme. The explicit centred-in-distance scheme

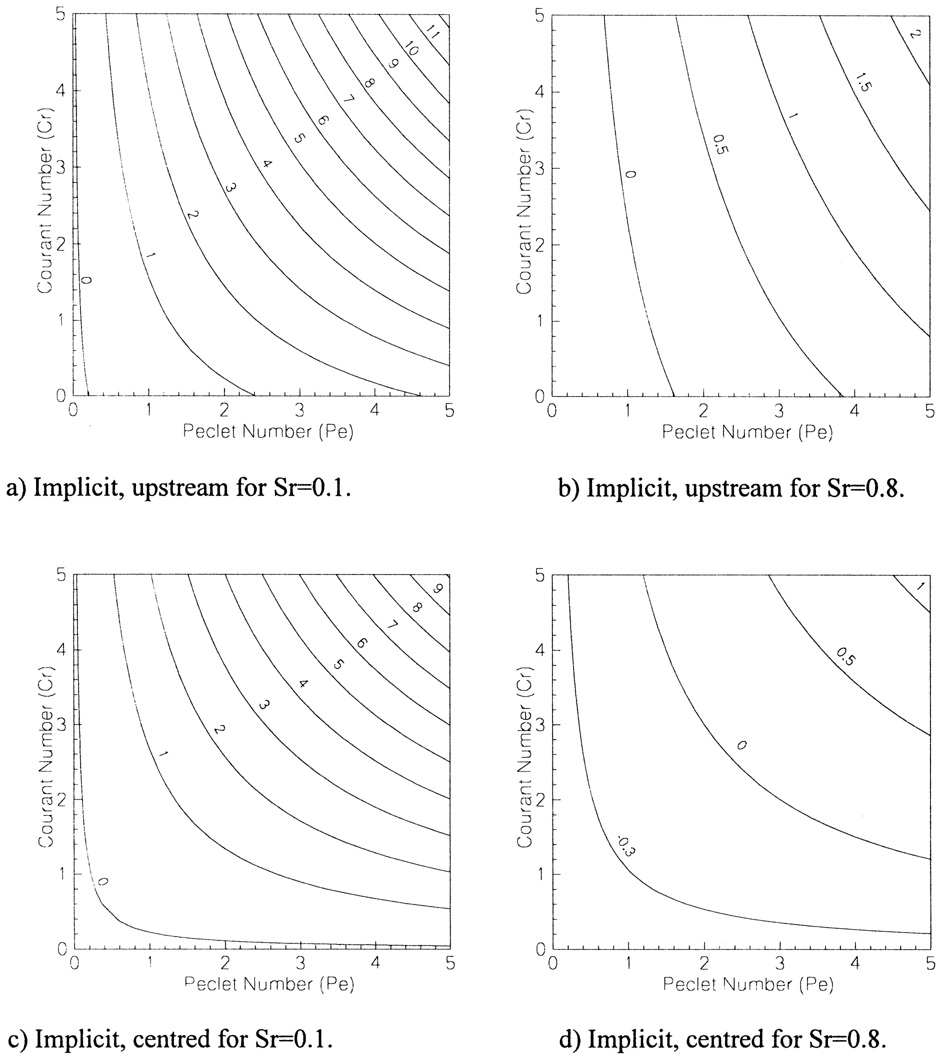


Fig. 6. Ratio of numerical dispersion coefficient to physical dispersion coefficient for implicit schemes. (a) explicit, upstream (b) explicit, centred.

shows less error than the other explicit scheme, though an improvement in results by correcting for truncation errors is still seen in Fig. 7b. The cumulative absolute value of errors for the explicit upstream and centred without the corrections are 0.35 and 0.07 mg l^{-1}, respectively. These values reduce to 0.03 and 0.008 mg l^{-1} when the correction is applied.

For the cases of the Crank-Nicolson schemes, a similar problem with $u = 25$ mm h^{-1}, $\Delta z = 20$ mm and $\Delta t = 5.0$ h is solved. In this case, the dimensionless numbers, Pe, Cr, and Sr, are 5, 6.25, and 0.5, respectively. Fig. 8 shows the results for the

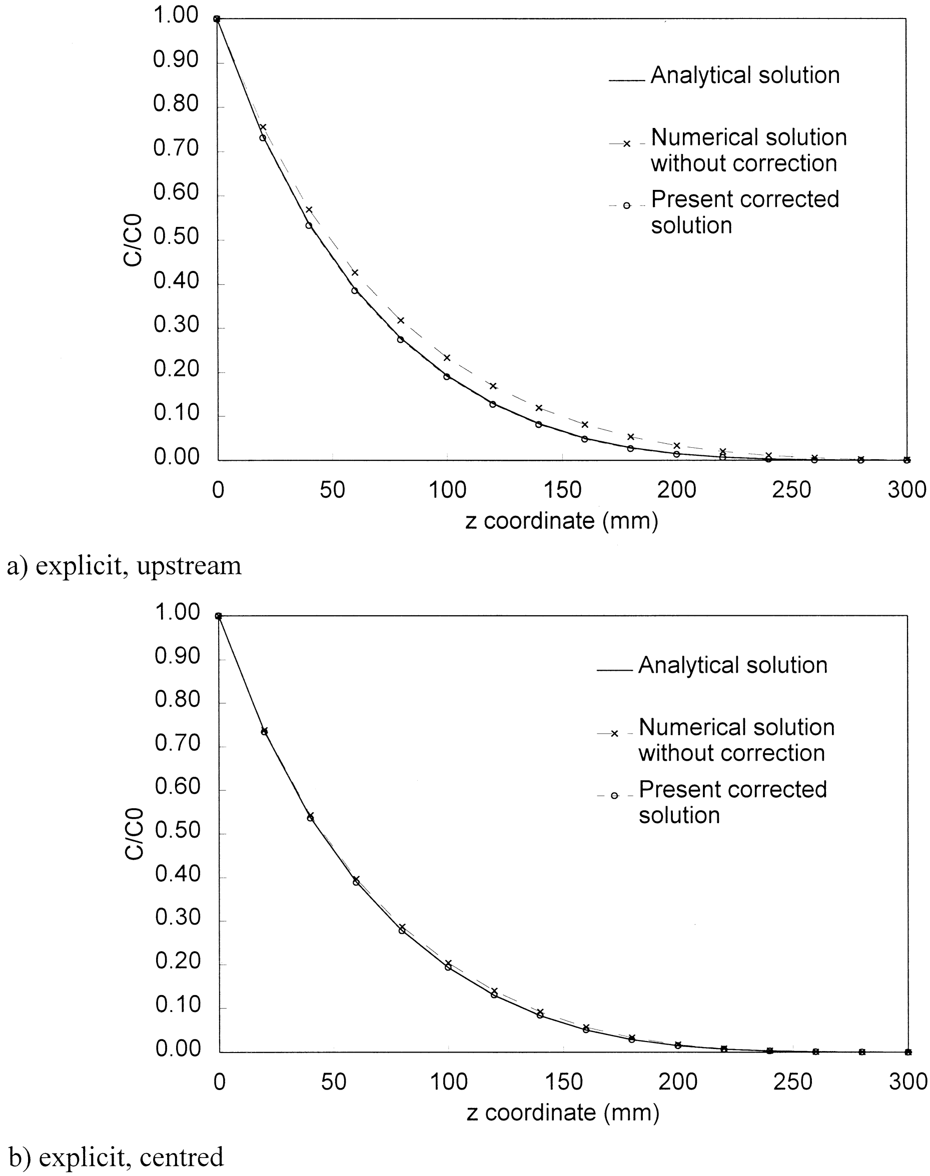
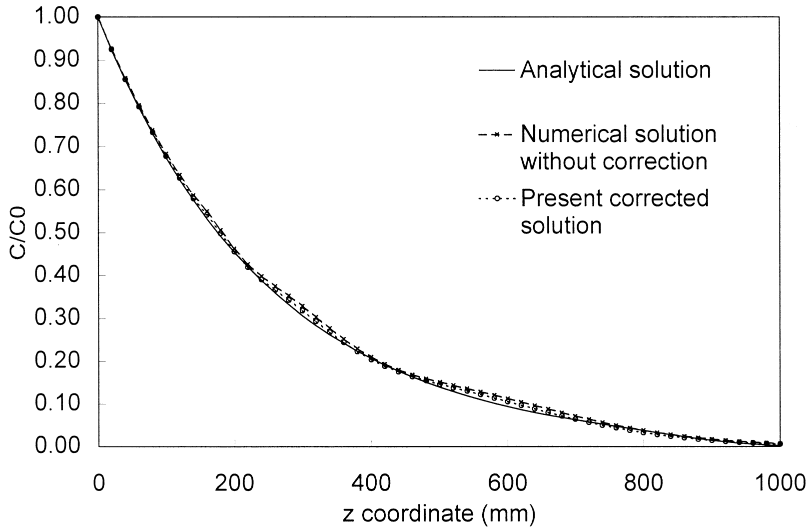
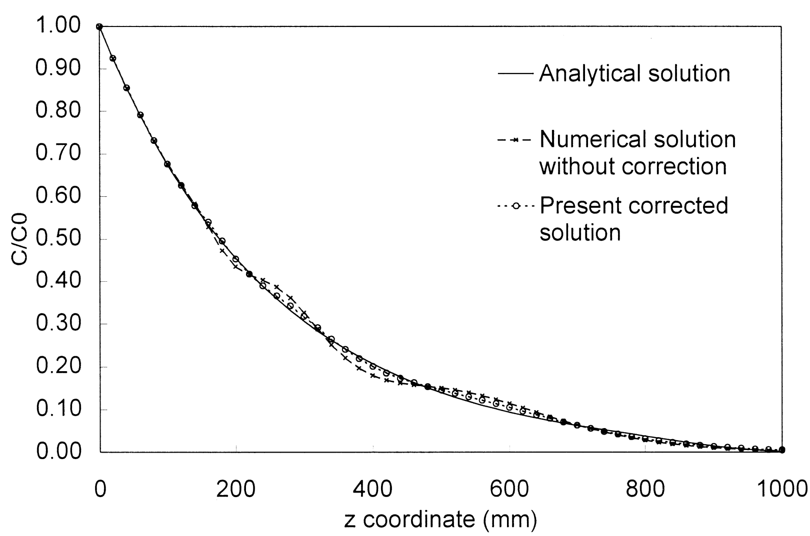


Fig. 7. Comparison of the analytical and numerical solutions after 20 hr: Pe = 1, Cr = 0.25, Sr = 0.1. (a) Crank–Nicolson, upstream (b) Crank–Nicolson, centred.

Crank–Nicolson schemes. As seen, the solutions based on the Crank–Nicolson schemes without the present correction oscillate around the analytical solution, because of the high value of the Peclet number in this case. As expected, the oscillation of the solution is more severe for the Crank–Nicolson centred-in-time scheme. Fig. 8 clearly illustrates



a) Crank-Nicolson, upstream



b) Crank-Nicolson, centred

Fig. 8. Comparison of the analytical and numerical solutions after 20 hr: Pe = 5, Cr = 6.25, Sr = 0.5.

that removing the truncation errors improves the results of the both Crank–Nicolson schemes and reduces the oscillation effects, especially for the Crank–Nicolson centred scheme. The cumulative absolute value of errors for the Crank-Nicolson upstream and centred without the corrections are 0.455 and 0.529 mg l^{-1}, respectively. These values reduce to 0.237 and 0.230 mg l^{-1} when the correction is applied.

6. Conclusions

The expressions for the truncation errors associated with the finite difference solution of the advection–dispersion equation with reaction are presented as functions of Peclet, Courant and the new Source/Sink dimensionless numbers. It is shown that all of the widely-used finite difference schemes have low order truncation errors, even the Crank–Nicolson with centred-in-distance approximation scheme. In fact, none of these methods has even zeroth order accuracy.

For small values of Sink/Source number, numerical dispersion increases as the Peclet and Courant numbers increase, except for the Crank-Nicolson upstream scheme where increasing the Courant number leads to a decrease in numerical dispersion. However, this trend is not observed for larger values of the Sink/Source number where no trend is observed between Sink/Source number and numerical dispersion. That is, an increase in Sink/Source number leads to an increase in error in some cases while in others it causes a decrease in the numerical dispersion value. The absolute values of numerical velocity and the reaction term increase for all schemes with increasing values of the Sink/Source number.

The effect of these truncation errors on the solution of an advection–dispersion equation with a first order reaction term are demonstrated for a case with a known analytical solution. Comparison shows that these errors are not negligible and that correcting the finite difference scheme for them results in a more accurate solution. The correction method will be especially useful when an accurate assessment of the solute concentration profile is needed such as in parameter estimation studies and in providing source terms for large-scale groundwater models.

Acknowledgements

The postgraduate scholarship of the Ministry of Culture and Higher Education of the Islamic Republic of Iran is appreciated. Financial assistance was provided partly by the Cooperative Research Centre for Ecological Sustainability of the Great Barrier Reef.

References

Ataie-Ashtiani, B., Lockington, D.A., Volker, R.E., 1995a. Comment on Integrated flux model for unsteady transport of trace organic chemicals in soils. Soil Sci. 159, 346–348.

Ataie-Ashtiani, B., Lockington, D.A., Volker, R.E., 1995b. Comment on removing numerically induced dispersion from finite difference models for solute and water transport in unsaturated soils. Soil Sci. 160, 442–443.

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

Chaudhari, N.M., 1971. An improved numerical technique for solving multidimensional miscible displacement equations. Soc. Petrol. Eng. J. 11, 277–284.

De Smedt, F., Wierenga, P.J., 1977. Simulation of water and solute transport in unsaturated soils. Proc. Third Int. Symp. Hydrology, Fort Collins.

Dudley, L.M., McLean, J.E., Furst, T.H., Jurinak, J.J., 1991. Sorption of cadmium copper from an acid mine waste extract by two calcareous soils: column studies. Soil Sci. 151, 121–135.

Konikow, L.F., Bredehoeft, J.D., 1978. Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water. U.S. Geological Survey Water-Resources Investigations Book 7, Chap. C2, 90 pp.
Lantz, R.B., 1971. Quantitative evaluation of numerical diffusion (truncation error). Soc. Petrol. Eng. J. 11, 315–320.
Moldrup, P., Yamaguchi, T., Hansen, J.Aa., Rolston, E., 1992. An accurate and numerically stable model for one-dimensional solute transport in soils. Soil Sci. 153, 261–273.
Moldrup, P., Yamaguchi, T., Rolston, D.E., Vestergaard, K., Hansen, J.Aa., 1994a. Removing numerically induced dispersion from finite difference models for solute and water transport in unsaturated soils. Soil Sci. 157, 153–161.
Moldrup, P., Poulsen, T.G., Rolston, D.E., Yamaguchi, T., Hansen, J.Aa., 1994b. Integrated flux model for unsteady transport of trace organic chemicals in soils. Soil Sci. 157, 137–152.
Moldrup, P., Kruse, C.W., Yamaguchi, T., Rolston, D.E., 1996. Modelling diffusion and reaction in soils: I. A diffusion and reaction corrected finite difference calculation scheme. Soil Sci. 161, 347–354.
Notodarmojo, S., Ho, G.E., Scott, W.D., Davis, G.B., 1991. Modelling phosphorus transport in soils and groundwater with two-consecutive reactions. Water Research 25, 1205–1216.
Smith, G.D., 1978. Numerical Solution of Partial Differential Equations: Finite Difference Methods, 2nd edn. Oxford Univ. Press, Oxford.
van Genuchten, M.Th., Gray, W.G., 1978. Analysis of some dispersion corrected numerical schemes for solution of the transport equation. Int. J. Num. Methods Eng. 12, 387–404.
van Genuchten, M.Th., Alves, W.J., 1982. Analytical Solutions of the One-Dimensional Convective–Dispersive Solute Transport Equation. US Dept. of Agriculture, Tech. Bull. No. 1661. 155 pp.
Zheng, C., 1990. MT3D: A Modular Three-dimensional Transport Model for Simulation of Advection, Dispersion and Chemical Reactions of Contaminants in Groundwater Systems. Report to the U.S. Environmental Protection Agency, Ada, OK, 170 pp.