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Numerical errors of explicit finite difference approximation for two-dimensional solute transport equation with linear sorption

B. Ataie-Ashtiani*, S.A. Hosseini

Department of Civil Engineering, Sharif University of Technology, P.O. Box 11365-9313, Tehran, Iran

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Abstract

The numerical errors associated with explicit upstream finite difference solutions of two-dimensional advection–dispersion equation with linear sorption are formulated from a Taylor analysis. The error expressions are based on a general form of the corresponding difference equation. The numerical truncation errors are defined using Peclet and Courant numbers in the X and Y direction, a sink/source dimensionless number and new Peclet and Courant numbers in the XY plane. The effects of these truncation errors on the explicit solution of a two-dimensional advection–dispersion equation with a first-order reaction or degradation are demonstrated by comparison with an analytical solution in uniform flow field. The results show that these errors are not negligible and correcting the finite difference scheme for them results in a more accurate solution.

Keywords: Advection—Dispersion-Reaction equation; Numerical methods; Finite Difference Model; Truncation errors

1. Introduction

The finite-difference method is a well-known numerical method that has been applied to the advection–dispersion equation (ADE) as discussed in many standard books on the subject (e.g. Zheng and Bennett, 2002). While there are many numerical investigations of the advection–dispersion equation, comparatively few studies have been devoted to the more general advection–dispersion–reaction equation. This equation arises in modeling heat and contaminant transport (e.g. Freijera et al., 1998; Stanbro, 2000; Islam and Singhal, 2002; Cokca, 2003).

Approximating differential equations in finite difference (FD) 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. Lantz (1971) and Chaudhari (1971) quantified numerical dispersion as a second-order error term through examination 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 (De Smedt and Wierenga, 1977; Van Genuchten and Gray, 1978; Notodarmojo et al., 1991; Dudley et al., 1991).

The numerical dispersion is the only truncation error for the case of ADE; nevertheless, for the more general transport equation (e.g. with reaction) other truncation errors are also introduced. Ataie-Ashtiani et al. (1995a) quantified the zero- and first-order truncation errors in the ADE with reaction (ADER) for the first time. 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

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* Corresponding author. Fax: +98-21-601-4828.
E-mail address: ataie@sharif.edu (B. Ataie-Ashtiani).

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Nomenclature

C	solute concentration [M L^{-3}]
C_0	initial concentration in inflow boundary [M L^{-3}]
Cr_{xx}	principal-term of Courant number [–]
Cr_{yy}	principal-term of Courant number [–]
Cr_{xy}	cross-term of Courant number [–]
D_{xx}	principal term of dispersion coefficient [L^2 T^{-1}]
D_{yy}	principal term of dispersion coefficient [L^2 T^{-1}]
D_{xy}	cross term of dispersion coefficient [L^2 T^{-1}]
$D_{\text{num}xx}$	principal term of numerical dispersion coefficient [L^2 T^{-1}]
$D_{\text{num}yy}$	principal term of numerical dispersion coefficient [L^2 T^{-1}]
$D_{\text{num}xy}$	cross term of numerical dispersion coefficient [L^2 T^{-1}]
erfc	complementary error function [–]
exp	exponential [–]
k	first-order reaction rate coefficient [T^{-1}]
k_{num}	numerical first-order reaction rate coefficient [T^{-1}]
Pe_{xx}	principal-term of Peclet number [–]
Pe_{xy}	cross-term of Peclet number [–]
Pe_{yy}	principal-term of Peclet number [–]
Sr	sink/source number [–]
t	time [T]
v	uniform flow velocity [L T^{-1}]
v_x	velocity component in X direction [L T^{-1}]
v_y	velocity component in Y direction [L T^{-1}]
$v_{\text{num}x}$	numerical velocity component in X direction [L T^{-1}]
$v_{\text{num}y}$	numerical velocity component in Y direction [L T^{-1}]
Y_1	y-coordinate of lower limit of solute source at $x = 0$ [L]
Y_2	y-coordinate of upper limit of solute source at $x = 0$ [L]
Δx	length increment in X direction [L]
Δy	length increment in Y direction [L]
Δt	time increment [T]
α_{L}	longitudinal dipersivity [L]
α_{T}	transverse dipersivity [L]
Σ	summation [–]
α	spatial weighting parameter in X direction [–]
β	spatial weighting parameter in Y direction [–]
θ	angle between local and global coordinate axis [–]

errors of the explicit centered 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.

Ataie-Ashtiani et al. (1999) derived the analytical expressions for truncation errors of general FD form of the one-dimensional ADER that covered explicit, Crank–Nicolson, and implicit schemes. They showed that none of the widely used FD schemes had second order accuracy for solving the ADER.

Many studies have been published for finite difference solution of the two-dimensional ADE (e.g. Konikow and Bredehoeft, 1978; Lappala et al., 1987; Healy, 1990; Sheu et al., 2000; Zheng and Bennett, 2002), but the authors are not aware of any studies of the truncation errors of the finite difference solution of the ADER in two-dimensions. The primary objectives of this paper are to derive the analytical expressions for truncation errors of the explicit upstream FD form of two-dimensional ADER and show how removing this truncation error improves the results. Dimensionless numbers are introduced and applied to define the numerical truncation errors.

The explicit method is extremely simple to implement in a computer code. This scheme has been implemented in a number of commonly used transport simulation models, e.g. the MOC code by Konikow and Bredehoeft (1978) and the MT3D code by Zheng (1990). The limitation of an explicit scheme is that there is a certain stability criterion associated with it, so that the size of time step cannot exceed a certain value. However, the use of an explicit scheme is efficient that it saves a large amount of computer memory that would be required by a matrix solver used in an implicit scheme. In addition, transport simulation has additional accuracy requirements, which limit the time step even without stability criterion (e.g. many advection-dominated problems). It should be noted that explicit calculation could be implemented conveniently in a mixed Eulerian–Lagrangian code such as MOC and MT3D (Zheng and Bennett, 2002).

2. Finite difference approximation of ADER

The two-dimensional advection–dispersion equation with a linear sorption (first order reaction) is written as:

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

where C is dissolved concentration [ML^{-3}], k is first-order reaction rate coefficient [T^{-1}], D_{xx}, D_{yy} are principal terms of dispersion coefficient [$L^2\ T^{-1}$], D_{xy} is cross-term of dispersion coefficient [$L^2\ T^{-1}$], v_x, v_y are velocity component in X and Y directions [$L\ T^{-1}$].

The general form of explicit FD approximation of Eq. (1), using α and β as spatial weighting parameters in X and Y directions may be expressed as:

$$\begin{aligned}\frac{C_{i,j}^{n+1}-C_{i,j}^{n}}{\Delta t}=&D_{xx}\left[\frac{C_{i+1,j}^{n}-2C_{i,j}^{n}+C_{i-1,j}^{n}}{\Delta x^2}\right]\\&+D_{yy}\left[\frac{C_{i,j+1}^{n}-2C_{i,j}^{n}+C_{i,j-1}^{n}}{\Delta y^2}\right]\\&+D_{xy}\left[\frac{C_{i+1,j+1}^{n}-C_{i+1,j-1}^{n}-C_{i-1,j+1}^{n}+C_{i-1,j-1}^{n}}{4\Delta x\Delta y}\right]\\&-v_x\left[\frac{(1-\alpha)C_{i,j}^{n}+\alpha C_{i+1,j}^{n}-(1-\alpha)C_{i-1,j}^{n}-\alpha C_{i,j}^{n}}{\Delta x}\right]\\&-v_y\left[\frac{(1-\beta)C_{i,j}^{n}+\beta C_{i,j+1}^{n}-(1-\beta)C_{i,j-1}^{n}-\beta C_{i,j}^{n}}{\Delta y}\right]\\&-kC_{i,j}^{n}\end{aligned}\tag{2}$$

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

The explicit FD scheme reduces to centered-in-space when $\alpha=\beta=0.5$ (the most obvious choice of α and β). An alternative spatial weighting scheme is the upstream or upwind scheme with positive velocity ($v_x, v_y > 0$) when $\alpha=\beta=0$ or with negative velocity ($v_x, v_y < 0$) when $\alpha=\beta=1.0$.

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 (Zheng and Bennett, 2002). The problem of artificial oscillation can be overcome through the use of upstream weighting. Upstream weighting tends to aggravate the numerical dispersion therefore explicit upstream method was selected for studying truncation errors. Then the simplified form of Eq. (2) for the case of $\alpha=\beta=0$ can be written as follows:

$$\begin{aligned}\frac{C_{i,j}^{n+1}-C_{i,j}^{n}}{\Delta t}=&D_{xx}\left[\frac{C_{i+1,j}^{n}-2C_{i,j}^{n}+C_{i-1,j}^{n}}{\Delta x^2}\right]\\&+D_{yy}\left[\frac{C_{i,j+1}^{n}-2C_{i,j}^{n}+C_{i,j-1}^{n}}{\Delta y^2}\right]\\&+D_{xy}\left[\frac{C_{i+1,j+1}^{n}-C_{i+1,j-1}^{n}-C_{i-1,j+1}^{n}+C_{i-1,j-1}^{n}}{4\Delta x\Delta y}\right]\\&-v_x\left[\frac{C_{i,j}^{n}-C_{i-1,j}^{n}}{\Delta x}\right]-v_y\left[\frac{C_{i,j}^{n}-C_{i,j-1}^{n}}{\Delta y}\right]-kC_{i,j}^{n}\end{aligned}\tag{3}$$

A Taylor series expansion of C about any grid point was used to determine the form of the truncation errors in one-dimension (Ataie-Ashtiani et al., 1999). If the same method is used for two-dimensional Taylor series expansion and the third and higher order spatial derivatives are neglected, as they are not present in the original equation, then

$$C_{i,j}^{n+1}=C_{i,j}^{n}+\sum_{m=1}^{\infty}\frac{\Delta t^m}{m!}\frac{\partial^m C}{\partial t^m}\tag{4}$$

$$C_{i+1,j}^{n}=C_{i,j}^{n}+\Delta x\frac{\partial C}{\partial x}+\frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2}+O(\Delta x^3)\tag{5}$$

$$C_{i-1,j}^{n}=C_{i,j}^{n}-\Delta x\frac{\partial C}{\partial x}+\frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2}+O(\Delta x^3)\tag{6}$$

$$\begin{aligned}C_{i\pm1,j\mp1}^{n}=&C_{i\pm1,j}^{n}\mp\Delta y\frac{\partial C}{\partial y}\Big|_{i\pm1,j}+\frac{\Delta y^2}{2}\frac{\partial^2 C}{\partial y^2}\Big|_{i\pm1,j}+O(\Delta y^3)\\=&C_{i,j}^{n}\pm\Delta x\frac{\partial C}{\partial x}+\frac{\Delta x^2}{2}\frac{\partial^2 C}{\partial x^2}\mp\Delta y\frac{\partial C}{\partial y}\\&+\frac{(\pm\Delta x)(\mp\Delta y)}{2}\frac{\partial^2 C}{\partial x\partial y}+\frac{\Delta y^2}{2}\frac{\partial^2 C}{\partial y^2}+O(\Delta x^3)\\&+O(\Delta y^3)+O(\Delta x^2\Delta y)+O(\Delta x\Delta y^2)\end{aligned}\tag{7}$$

$$C_{i,j+1}^{n}=C_{i,j}^{n}+\Delta y\frac{\partial C}{\partial y}+\frac{\Delta y^2}{2}\frac{\partial^2 C}{\partial y^2}+O(\Delta y^3)\tag{8}$$

$$C_{i,j-1}^{n}=C_{i,j}^{n}-\Delta y\frac{\partial C}{\partial y}+\frac{\Delta y^2}{2}\frac{\partial^2 C}{\partial y^2}+O(\Delta y^3)\tag{9}$$

The second and higher order temporal derivatives of C are written in terms of spatial derivatives of C using the differentiated from of Eq. (2), and again the third and higher order spatial derivatives (in X or Y directions) are neglected. It is noticed that the transport parameters are assumed constant only within each combination of time and depth increments in finite difference calculation. Thus

$$\begin{aligned}\frac{\partial^2 C}{\partial t^2}=&D_{xx}\frac{\partial^2}{\partial x^2}\left(\frac{\partial C}{\partial t}\right)+D_{yy}\frac{\partial^2}{\partial y^2}\left(\frac{\partial C}{\partial t}\right)\\&+D_{xy}\frac{\partial^2}{\partial x\partial y}\left(\frac{\partial C}{\partial t}\right)-v_x\frac{\partial}{\partial x}\left(\frac{\partial C}{\partial t}\right)\\&-v_y\frac{\partial}{\partial y}\left(\frac{\partial C}{\partial t}\right)-k\frac{\partial C}{\partial t}\\\approx&\left[-2kD_{xx}+v_x^2\right]\frac{\partial^2 C}{\partial x^2}+\left[-2kD_{yy}+v_y^2\right]\frac{\partial^2 C}{\partial y^2}\\&+\left[-2kD_{xy}+2v_xv_y\right]\frac{\partial^2 C}{\partial x\partial y}\\&+\left[2kv_x\right]\frac{\partial C}{\partial x}+\left[2kv_y\right]\frac{\partial C}{\partial y}+k^2C\end{aligned}\tag{10}$$

$$\begin{aligned}\frac{\partial^3 C}{\partial t^3} &= \left[3k^2D_{xx} - 3kv_x^2\right]\frac{\partial^2 C}{\partial x^2} + \left[3k^2D_{yy} - 3kv_y^2\right]\frac{\partial^2 C}{\partial y^2}\\ &\quad + \left[3k^2D_{xy} - 6kv_xv_y\right]\frac{\partial^2 C}{\partial x\partial y} + \left[-3k^2v_x\right]\frac{\partial C}{\partial x}\\ &\quad + \left[-3k^2v_y\right]\frac{\partial C}{\partial y} - k^3C \qquad (11)\end{aligned}$$

Similarly,

$$\begin{aligned}\frac{\partial^4 C}{\partial t^4} &= \left[-4k^3D_{xx} + 6k^2v_x^2\right]\frac{\partial^2 C}{\partial x^2}\\ &\quad + \left[-4k^3D_{yy} + 6k^2v_y^2\right]\frac{\partial^2 C}{\partial y^2}\\ &\quad + \left[-4k^3D_{xy} + 12k^2v_xv_y\right]\frac{\partial^2 C}{\partial x\partial y}\\ &\quad + \left[4k^3v_x\right]\frac{\partial C}{\partial x} + \left[4k^3v_y\right]\frac{\partial C}{\partial y} + k^4C \qquad (12)\end{aligned}$$

or in general, for $m \geq 2$;

$$\begin{aligned}\frac{\partial^m C}{\partial t^m} &= (-1)^m\left[-mk^{m-1}D_{xx} + \frac{m(m-1)}{2}k^{m-2}v_x^2\right]\frac{\partial^2 C}{\partial x^2}\\ &\quad + (-1)^m\left[-mk^{m-1}D_{yy} + \frac{m(m-1)}{2}k^{m-2}v_y^2\right]\frac{\partial^2 C}{\partial y^2}\\ &\quad + (-1)^m\left[-mk^{m-1}D_{xy} + m(m-1)k^{m-2}v_xv_y\right]\frac{\partial^2 C}{\partial x\partial y}\\ &\quad + (-1)^m\left[mk^{m-1}v_x\right]\frac{\partial C}{\partial x} + (-1)^m\left[mk^{m-1}v_y\right]\frac{\partial C}{\partial y}\\ &\quad + (-1)^m k^m C \qquad (13)\end{aligned}$$

Therefore Eq. (4) is written as:

$$\begin{aligned}C_{i,j}^{n+1} &= C_{i,j}^n + \Delta t\frac{\partial C}{\partial t} + \sum_{m=2}^{\infty}\frac{\Delta t^m}{(m-1)!}(-1)^m\\ &\quad \times\left\{\left[-k^{m-1}D_{xx} + \frac{(m-1)}{2}k^{m-2}v_x^2\right]\frac{\partial^2 C}{\partial x^2}\right.\\ &\quad + \left[-k^{m-1}D_{yy} + \frac{(m-1)}{2}k^{m-2}v_y^2\right]\frac{\partial^2 C}{\partial y^2}\\ &\quad + \left[-k^{m-1}D_{xy} + (m-1)k^{m-2}v_xv_y\right]\frac{\partial^2 C}{\partial x\partial y}\\ &\quad \left. + \left[k^{m-1}v_x\right]\frac{\partial C}{\partial x} + \left[k^{m-1}v_y\right]\frac{\partial C}{\partial y} + \frac{k^mC}{m}\right\} \qquad (14)\end{aligned}$$

Substituting Eqs. (5)–(9) and (14) in Eq. (2) gives:

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

3. Truncation error formulations in dimensionless form

A comparison between Eq. (15) and the original governing differential equation shows that discretization introduces three forms of truncation error. They can be identified as a second-order truncation error or numerical dispersion in X and Y directions, $D_{\mathrm{num}xx}$ and $D_{\mathrm{num}yy}$, and cross-term, $D_{\mathrm{num}xy}$:

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

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

$$\begin{aligned}D_{\mathrm{num}xy} &= -\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m\\ &\quad \times\left[-k^{m-1}D_{xy} + (m-1)k^{m-2}v_xv_y\right] \qquad (18)\end{aligned}$$

a first-order truncation error or numerical water velocity in X and Y directions, $v_{\mathrm{num}x}$ and $v_{\mathrm{num}y}$:

$$v_{\mathrm{num}x}=\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m k^{m-1}v_x \tag{19}$$

$$v_{\mathrm{num}y}=\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{(m-1)!}(-1)^m k^{m-1}v_y \tag{20}$$

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

$$k_{\mathrm{num}}=\sum_{m=2}^{\infty}\frac{\Delta t^{m-1}}{m!}(-1)^m k^m \tag{21}$$

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:

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

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

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

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

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

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

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

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

$$\frac{D_{\mathrm{num}xx}}{D_{xx}}=\frac{Pe_{xx}}{2}-\sum_{m=2}^{\infty}\frac{(-1)^m}{(m-1)!}\times\left[-Sr^{m-1}+\frac{(m-1)}{2}Sr^{m-2}Pe_{xx}Cr_{xx}\right] \tag{25}$$

$$\frac{D_{\mathrm{num}yy}}{D_{yy}}=\frac{Pe_{yy}}{2}-\sum_{m=2}^{\infty}\frac{(-1)^m}{(m-1)!}\times\left[-Sr^{m-1}+\frac{(m-1)}{2}Sr^{m-2}Pe_{yy}Cr_{yy}\right] \tag{26}$$

$$\frac{D_{\mathrm{num}xy}}{D_{xy}}=-\sum_{m=2}^{\infty}\frac{(-1)^m}{(m-1)!}\times\left[-Sr^{m-1}+(m-1)Sr^{m-2}Pe_{xy}Cr_{xy}\right] \tag{27}$$

$$\frac{v_{\mathrm{num}x}}{v_x}=\sum_{m=2}^{\infty}\frac{(-1)^m Sr^{m-1}}{(m-1)!} \tag{28}$$

$$\frac{v_{\mathrm{num}y}}{v_y}=\sum_{m=2}^{\infty}\frac{(-1)^m Sr^{m-1}}{(m-1)!} \tag{29}$$

$$\frac{k_{\mathrm{num}}}{k}=\sum_{m=2}^{\infty}\frac{(-1)^m Sr^{m-1}}{m!} \tag{30}$$

As seen, the second order truncation error or numerical dispersion has three expressions, two expressions in X, Y directions and one cross-term expression. Numerical dispersions in X and Y direction are similar to numerical dispersions of one-dimensional ADER (Ataie-Ashtiani et al., 1999). We present a new numerical dispersion ($D_{\mathrm{num}xy}$, cross-term numerical dispersion) that introduces new dimensionless numbers as Pe_{xy} and Cr_{xy}. Eq. (18) shows that $D_{\mathrm{num}xy}$ exists even if D_{xy} is equal to zero. The zero and first order truncation errors are similar to the one-dimensional case (Ataie-Ashtiani et al., 1999). The second order truncation error is a function of Pe and Cr and Sr numbers, but the zero and first-order truncation errors are only a function of Sr.

Eqs. (25)–(30) present $D_{\mathrm{num}xx}/D_{xx}$, $D_{\mathrm{num}yy}/D_{yy}$, $D_{\mathrm{num}xy}/D_{xy}$, $v_{\mathrm{num}x}/v_x$, $v_{\mathrm{num}y}/v_y$, k_{num}/k as infinite series. Ataie-Ashtiani et al. (1999) showed a maximum of four terms ($m=5$) of the series gives enough accuracy in the calculation of truncation errors in one-dimensional ADER. The same accuracy is obtained with four terms ($m=5$) of the series in two-dimensional ADER too. The ratio of numerical to physical dispersion coefficient in X and Y direction as function of Pe and Cr numbers in the same direction (X or Y) for two different values of Sr, 0.1 and 0.8, are illustrated in Figs. 1 and 2. In Figs. 3 and 4 the ratio of $D_{\mathrm{num}xy}/D_{xy}$ has been shown for two values of Sr, 0.1 and 0.8, as a function of cross-terms of Pe and Cr numbers (Pe_{xy} and Cr_{xy}). These results demonstrate the variation in numerical dispersion for two-dimensional ADER. Figs. 1–4 show that as the Peclet number increases, numerical dispersion increases in general (X or Y or XY), but as the Courant number increases, only cross-term of numerical dispersion increases. Therefore numerical dispersion in X and Y directions ($D_{\mathrm{num}xx}$, $D_{\mathrm{num}yy}$) have different behavior with respect to the cross-term of numerical dispersion ($D_{\mathrm{num}xy}$).

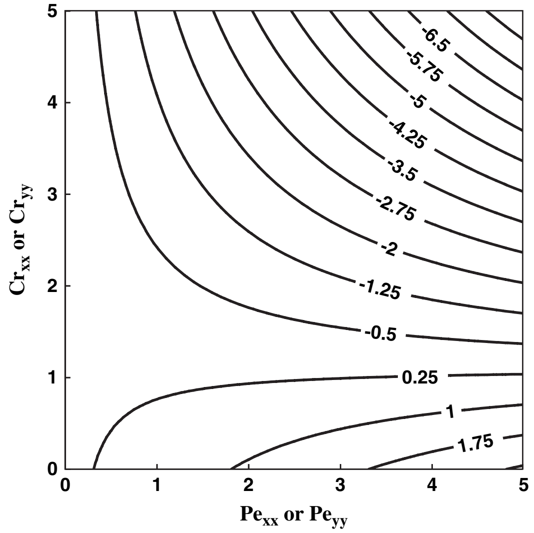

Fig. 1. Ratio of principal term of numerical dispersion coefficient to principal term of physical dispersion coefficient ($D_{\mathrm{num}xx}/D_{xx}$ or $D_{\mathrm{num}yy}/D_{yy}$) for $Sr = 0.1$.

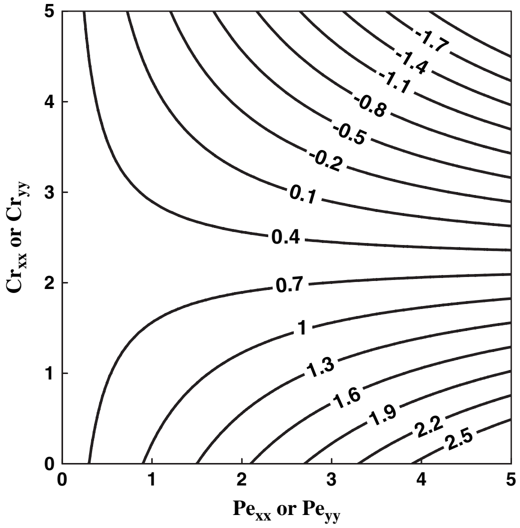

Fig. 2. Ratio of principal term of numerical dispersion coefficient to principal term of physical dispersion coefficient ($D_{\mathrm{num}xx}/D_{xx}$ or $D_{\mathrm{num}yy}/D_{yy}$) for $Sr = 0.8$.

In general, the truncation errors of upstream explicit FD discretization in one-, two- and three-dimensional ADER can be formulated as:

$$\begin{cases} \dfrac{D_{\mathrm{num}x_ix_j}}{D_{x_ix_j}} = \delta_{ij}\dfrac{Pe_{x_ix_j}}{2} - \displaystyle\sum_{m=2}^{\infty}\dfrac{(-1)^m}{(m-1)!} \\ \qquad\qquad \times\left[-Sr^{m-1} + \dfrac{(m-1)}{(1+\delta_{ij})}Sr^{m-2}Pe_{x_ix_j}Cr_{x_ix_j}\right] \\ \delta_{ij} = \begin{Bmatrix} 1 & i=j \\ 0 & i\neq j \end{Bmatrix} \qquad i=j=1,2,3 \end{cases} \tag{31}$$

$$\frac{v_{\mathrm{num}x_i}}{v_{x_i}} = \sum_{m=2}^{\infty}\frac{(-1)^m Sr^{m-1}}{(m-1)!} \tag{32}$$

$$\frac{k_{\mathrm{num}}}{k} = \sum_{m=2}^{\infty}\frac{(-1)^m Sr^{m-1}}{m!} \tag{33}$$

Also based on the comparison between Peclet and Courant numbers in one and two dimensions, we can define these dimensionless numbers in general as:

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

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

Similar to Ataie-Ashtiani et al. (1996, 1999), the stability criteria of explicit upstream scheme for two-dimensional ADER is determined using matrix method of Smith (1978). Using the matrix method the stability criteria is determined as follows:

$$\Delta t \leq \frac{1}{\dfrac{2D_{xx}}{\Delta x^2} + \dfrac{2D_{yy}}{\Delta y^2} + \dfrac{v_x}{\Delta x} + \dfrac{v_y}{\Delta y} + \dfrac{k}{2}} \tag{36}$$

4. Removing truncation errors

The effect of zero-, first- and second order truncation errors on the results of the explicit upstream scheme is illustrated here. The explicit schemes are well-known because of its simplicity. To remove the induced

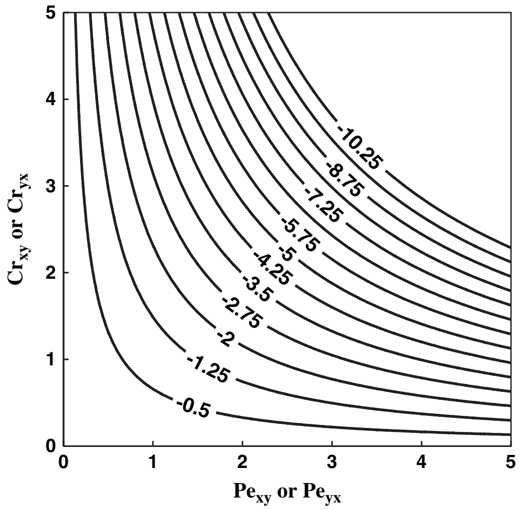

Fig. 3. Ratio of cross term of numerical dispersion coefficient to cross term of physical dispersion coefficient ($D_{\mathrm{num}xy}/D_{xy}$ or $D_{\mathrm{num}yx}/D_{yx}$) for $Sr = 0.1$.

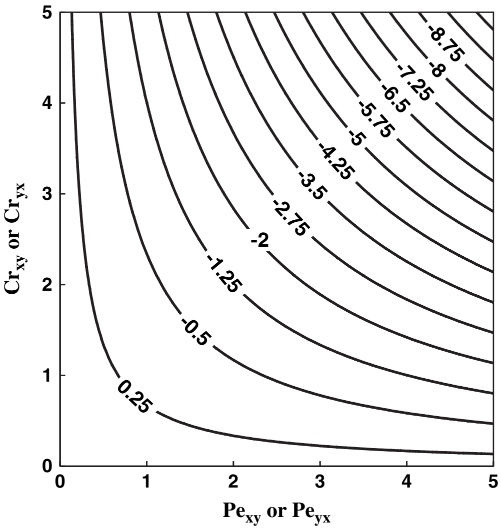

Fig. 4. Ratio of cross term of numerical dispersion coefficient to cross term of physical dispersion coefficient ($D_{\text{num}xy}/D_{xy}$ or $D_{\text{num}yx}/D_{yx}$) for $Sr = 0.8$.

numerical truncation errors from the upstream finite difference model, Eq. (3) is rewritten as:

$$\begin{aligned}
&\frac{C_{i,j}^{n+1}-C_{i,j}^{n}}{\Delta t}\\
&= D_{xx}^{*}\left[\frac{C_{i+1,j}^{n}-2C_{i,j}^{n}+C_{i-1,j}^{n}}{\Delta x^{2}}\right]\\
&\quad + D_{yy}^{*}\left[\frac{C_{i,j+1}^{n}-2C_{i,j}^{n}+C_{i,j-1}^{n}}{\Delta y^{2}}\right]\\
&\quad + D_{xy}^{*}\left[\frac{C_{i+1,j+1}^{n}-C_{i-1,j+1}^{n}-C_{i+1,j-1}^{n}+C_{i-1,j-1}^{n}}{4\Delta x\Delta y}\right]\\
&\quad - v_{x}^{*}\left[\frac{C_{i,j}^{n}-C_{i-1,j}^{n}}{\Delta x}\right]-v_{y}^{*}\left[\frac{C_{i,j}^{n}-C_{i,j-1}^{n}}{\Delta y}\right]-k^{*}C_{i,j}^{n}
\end{aligned} \tag{37}$$

where $D_{xx}^{*} = D_{xx} - D_{\text{num}xx}$, $D_{yy}^{*} = D_{yy} - D_{\text{num}yy}$, $D_{xy}^{*} = D_{xy} - D_{\text{num}xy}$, $v_{x}^{*} = v_{x} - v_{\text{num}x}$, $v_{y}^{*} = v_{y} - v_{\text{num}y}$, $k^{*} = k - k_{\text{num}}$.

The effect of zero, first and second order truncation errors on the results of the explicit upstream FD scheme is assessed by comparing the FD model results with the analytical solution for two-dimensional ADER in uniform flow by Wexler (1991). Solutions for one-dimensional solute-transport equation for variety of boundary and initial conditions are given in Van Genuchten and Alves (1982). Fewer analytical solutions have been published for the two- and three-dimensional forms of the solute transport equation. Wexler (1991) 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, so the analytical solution is given for this equation:

$$\frac{\partial C}{\partial t} = D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} - v\frac{\partial C}{\partial x} - kC \tag{38}$$

Wexler (1991) presented an analytical solution for semi-infinite aquifer of infinite width with a strip source for the following initial and boundary conditions.

Boundary conditions:

$$C = C_0, \quad x = 0 \text{ and } Y_1 < y < Y_2 \tag{39a}$$

$$C = 0, \quad x = 0 \text{ and } y < Y_1 \text{ or } y > Y_2 \tag{39b}$$

$$C, \frac{\partial C}{\partial y} = 0, \quad y = \pm\infty \tag{39c}$$

$$C, \frac{\partial C}{\partial x} = 0, \quad x = \infty \tag{39d}$$

Initial condition:

$$C = 0, \; 0 < x < \infty \text{ and } -\infty < y < +\infty \text{ at } t = 0 \tag{40}$$

where Y_1 is y-coordinate of lower limit of solute source at $x = 0$ [L], Y_2 is y-coordinate of upper limit of solute source at $x = 0$ [L], C_0 is solute concentration at inflow boundary [M L^{-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 coefficients (D_{xx}, D_{yy}) are constant.

Wexler (1991) presented the following analytical solution for Eq. (38):

$$\begin{aligned}
C(x,y,t) = &\frac{C_0 x}{4\sqrt{\pi D_{xx}}}\exp\left[\frac{vx}{2D_{xx}}\right]\\
&\int_{\tau=0}^{\tau=t} \tau^{-3/2}\exp\left[-\left(\frac{v^2}{4D_{xx}}+k\right)\tau - \frac{x^2}{4D_{xx}\tau}\right]\\
&\cdot\left\{\operatorname{erfc}\left[\frac{(Y_1 - y)}{2\sqrt{D_{yy}\tau}}\right] - \operatorname{erfc}\left[\frac{(Y_2 - y)}{2\sqrt{D_{yy}\tau}}\right]\right\}\mathrm{d}\tau
\end{aligned} \tag{41}$$

This analytical solution can be used when the line source is along the Y coordinate and constant velocity vector is perpendicular to it. Numerical solution is obtained in global coordinate system ($X-Y$) with the line source along any direction and constant velocity vector perpendicular to it. Analytical solution is obtained in a local coordinate system ($X' - Y'$) with line source along the Y'coordinate. Dispersion coefficients and velocity components in two different coordinate systems (global and local) change according to Eqs. (42)–(46) (Zheng and Bennett, 2002).

$$D_{xx} = \alpha_L \frac{v_x^2}{|v|} + \alpha_{\mathrm{T}} \frac{v_y^2}{|v|} \tag{42a}$$

$$D_{x'x'} = \alpha_{\mathrm{L}} \frac{v_{x'}^2}{|v|} + \alpha_{\mathrm{T}} \frac{v_{y'}^2}{|v|} \tag{42b}$$

$$D_{yy} = \alpha_{\mathrm{L}} \frac{v_y^2}{|v|} + \alpha_{\mathrm{T}} \frac{v_x^2}{|v|} \tag{43a}$$

$$D_{y'y'} = \alpha_{\mathrm{L}} \frac{v_{y'}^2}{|v|} + \alpha_{\mathrm{T}} \frac{v_{x'}^2}{|v|} \tag{43b}$$

$$D_{xy} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}}) \frac{v_x v_y}{|v|} \tag{44a}$$

$$D_{x'y'} = (\alpha_{\mathrm{L}} - \alpha_{\mathrm{T}}) \frac{v_{x'} v_{y'}}{|v|} \tag{44b}$$

$$\begin{bmatrix} v_x \\ v_y \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} v_{x'} \\ v_{y'} \end{bmatrix} \tag{45}$$

$$|v| = \sqrt{v_x^2 + v_y^2} = \sqrt{v_{x'}^2 + v_{y'}^2} \tag{46}$$

where θ is angle between local and global coordinate axis and α_{L} [L] and α_{T} [L] are longitudinal and transverse dispersity, respectively. It should be noted prime parameters refer to local coordinate system ($X' - Y'$). In the local coordinate system, we have only one component of velocity ($v_{x'} = v$ and $v_{y'} = 0$) so the dispersion coefficients and velocity components are simplified as follows:

$$D_{x'x'} = \alpha_{\mathrm{L}} v \tag{47a}$$

$$D_{y'y'} = \alpha_{\mathrm{T}} v \tag{47b}$$

$$D_{x'y'} = 0 \tag{47c}$$

Therefore for the local system we can use the above analytical solution (Eq. (41)). Transformation from the local system to the global system is achieved according to Eq. (48). It should be noticed that for the analytical solution there is no solute concentration behind the source line; however for the numerical solution it exists due to dispersion so the results are compared in the region at the front of the source line.

$$\begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} X' \\ Y' \end{bmatrix} \tag{48}$$

A square medium is considered with the parameter values of $v_{x'} = 20.0$ mm h^{-1}, $v_{y'} = 0.0$, $v_y = v_x = 10\sqrt{2}$ mm h^{-1}, $D_{x'x'} = 100.0$ mm^2 h^{-1}, $D_{y'y'} = 50.0$ mm^2 h^{-1}, $D_{xx} == D_{yy} = 75.0$ mm^2 h^{-1}, $D_{xy} = 25.0$ mm^2 h^{-1}, $k = 0.01$ h^{-1}, and C_0 is taken as 1000.0 mg l^{-1}. This problem is solved with $\Delta x = \Delta y = 10\sqrt{2}$ mm, $\Delta x' = \Delta y' = 20.0$ mm and $\Delta t = 0.2$ h. Constant longitudinal and transverse dispersity for this problem are 5.0 and 2.5 mm, respectively. Therefore the dimensionless numbers, Pe_{xx}, Pe_{xy}, Pe_{yy}, Cr_{xx}, Cr_{xy}, Cr_{yy}, $Pe_{x'x'}$, $Pe_{x'y'}$, $Pe_{y'y'}$, $Cr_{x'x'}$, $Cr_{x'y'}$, $Cr_{y'y'}$, and Sr for this case are 2.67, 4.0, 2.67, 0.2, 0.2, 0.2, 4, 0, 0, 0.2, 0, 0 and 0.002, respectively.

Fig. 5 shows four contour levels of 0.15, 0.4, 0.65, and 0.9 of C/C_0, in $X-Y$ plane for the analytical solution and numerical solution in the cases without correction and with correction for truncation errors. Fig. 6 shows the normalized concentration ratio, C/C_0, parallel to line source (perpendicular to centerline of plume) at distance of 500.0 mm from line source for the analytical and numerical solutions with and without correction. The cumulative absolute value of errors without correction is 2640.0 mg l^{-1}. This value reduces to 805 mg/lit when the correction is applied.

Fig. 7 illustrates the concentration ratio, C/C_0, along centerline of plume for the analytical and numerical solutions with and without correction. Fig. 8 shows the time series of concentration ratio, C/C_0, at point of intersection of two lines that are shown in Figs. 6 and 7, with and without correction for truncation errors. As shown in all of these figures (Figs. 6–8), the difference between numerical solutions with and without correction is considerable and including the corrections

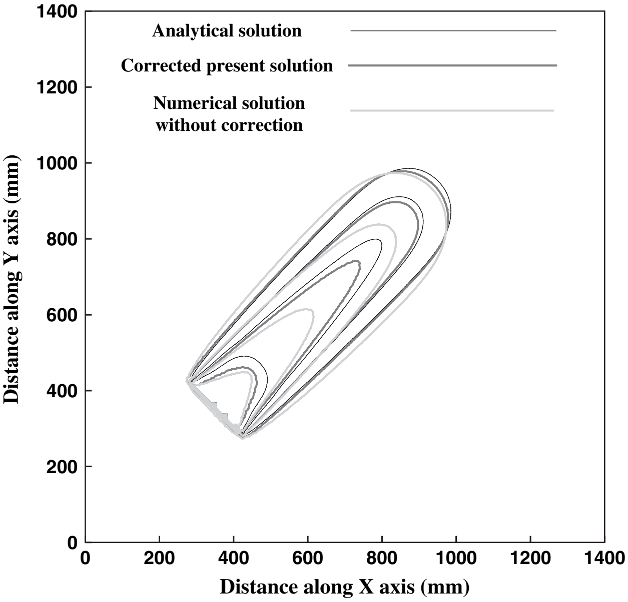

Fig. 5. Concentration distribution of line source for analytical and numerical solution 40.0 h after injection.

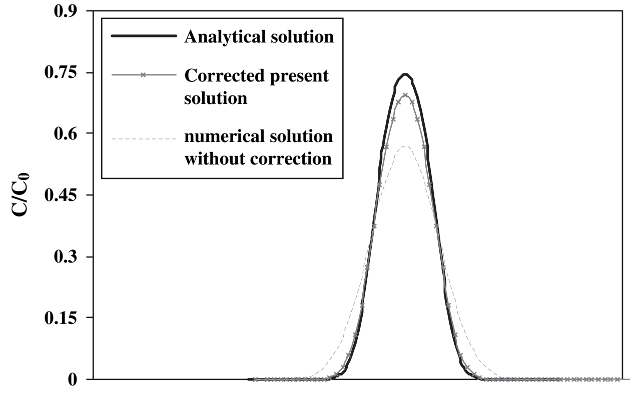

Fig. 6. Concentration distribution for analytical and numerical solution parallel to line source at 500.0 mm from line source 40 h after injection.

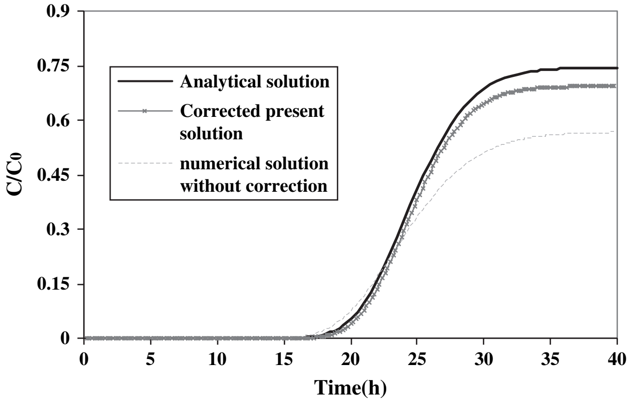

Fig. 8. Analytical and numerical solution for concentration at point in the domain of influence of plume.

significantly improves the numerical results. These cases show that corrections for truncation errors are effective in improving the results of the explicit FD scheme.

5. Conclusion

In this work we have determined the expressions for the truncation errors associated with the upstream explicit finite difference solution of two-dimensional advection–dispersion equation with first-order reaction or degradation. These truncation errors are presented as a function of principal- and cross-term of Peclet and Courant and sink/source dimensionless numbers.

Comparison of truncation errors between one- and two-dimensional ADER show that second-order truncation errors have a matrix form as matrix of dispersion coefficient, first-order truncation errors have a vector form similar to velocity vector, and zero-order truncation error is independent of dimensions of ADER.

Zero-order truncation error becomes zero if the first-order reaction rate coefficient equals zero. Similarly, if one component of velocity vector is zero, then the first-order truncation error becomes zero in the same direction, but if the principal and cross terms of physical dispersion are zero, the second-order truncation error or numerical dispersion may be formed.

In an upstream explicit FD scheme, principal and cross-terms of numerical dispersion increase with the increase of Peclet, Courant and sink/source numbers. Moreover, the absolute value of numerical velocity vector component and reaction term increase with increase in sink/source number.

New cross-axial Peclet and Courant numbers in two dimensions, Pe_{xy} and Cr_{xy}, are defined. The effect of these truncation errors on the solution of two-dimensional advection–dispersion equation with first-order reaction terms is demonstrated for a case with a known analytical solution. It is shown that these errors are not negligible, and removing them can significantly improve the numerical result and produce a more accurate numerical solution.

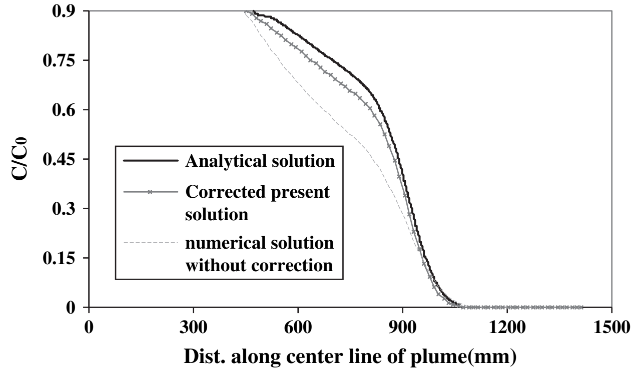

Fig. 7. Concentration distribution for analytical and numerical solution along center line of plume 40 h after injection.

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