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

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

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

Keywords: Advection–dispersion–reaction equation; Numerical method; Finite difference method; Truncation errors

1. Introduction

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

There are many numerical investigations of advection–dispersion equation (transport equation). However, a few studies have been devoted to the more general advection–dispersion–reaction equation (ADRE). The numerical solution of ADRE has its complexity because of the reaction term. The reaction term accounts for degradation or adsorption, this term can cause numerical instability problems. Ongoing research effort in this area reflects difficulty in solving the ADE by numerical methods for the cases such as advection-dominated problems, where the hyperbolic behavior of this equation is problematic especially in multi-dimensional ADE [1,2]. Also the solution of the transport equation (for advection-dominated problems), by many standard numerical procedures is plagued to some degree by two types of numerical problems. The first type is numerical dispersion due to the discretization of the governing equation. The second type of numerical problem is artificial oscillation [3].

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

* Corresponding author. Fax: +98 21 601 4828.
E-mail addresses: ataie@sharif.edu (B. Ataie-Ashtiani), hoseyni@mehr.sharif.edu (S.A. Hosseini).

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Nomenclature

C	solute concentrations [M L^{-3}]
C_0	solute concentration in injected fluid [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}]
$D_{\mathrm{num}xx}$	principal-term of numerical dispersion coefficient [L^{2}T^{-1}]
$D_{\mathrm{num}yy}$	principal-term of numerical dispersion coefficient [L^{2}T^{-1}]
$D_{\mathrm{num}xy}$	cross-term of numerical dispersion coefficient [L^{2}T^{-1}]
erfc	complimentary 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}]
$v_{\mathrm{num}x}$	numerical velocity component in X direction [L T^{-1}]
$v_{\mathrm{num}y}$	numerical velocity component in Y direction [L T^{-1}]
Δx	length increment in X direction [L]
Δy	length increment in Y direction [L]
Δt	time increment [T]
$\sum$	summation [–]
α_i	spatial weighting parameter in i direction [–]

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

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

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

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

Approximating differential equations in finite difference models by discretization introduces numerical errors (truncation error). In the case of transport equations like the advection–dispersion equation, numerical dispersion is a well-known consequence of truncation error [3,11, 20,21]. Lantz [20] and Chaudhari [21] quantified numerical dispersion as a second-order error through 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 [1,22–27]. Notodarmojo et al. [24] presented a numerical model for phosphorus transport in soils and ground water with two-consecutive reactions. The model uses an explicit FD scheme and takes into account the influence of numerical dispersion although the effects of zero- and first-order truncation errors are neglected. Noye et al. discussed on the modified equivalent partial differential equation (MEPDE) truncation errors and estimated the accuracy of FDMs based on artificial damping and phase shifting property. They also compared amplitude response and relative wave speed obtained in a series form using the coefficients of MEPDE to examine the accuracy of different FDMs [26,27].

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

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