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Numerical solution of unsteady advection dispersion equation arising in contaminant transport through porous media using neural networks

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ABSTRACT

A soft computing approach based on artificial neural network (ANN) and optimization is presented for the numerical solution of the unsteady one-dimensional advection–dispersion equation (ADE) arising in contaminant transport through porous media. A length factor ANN method, based on automatic satisfaction of arbitrary boundary conditions (BCs) was chosen for the numerical solution of ADE. The strength of ANN is exploited to construct a trial approximate solution (TAS) for ADE in a way that it satisfies the initial or BCs exactly. An unsupervised error is constructed in approximating the solution of ADE which is minimized by training ANN using gradient descent algorithm (GDA). Two challenging test problems of ADE are considered in this paper, in which, the first problem has steep boundary layers near $x = 1$ and many numerical methods create non-physical oscillation near steep boundaries. Also for the second problem many numerical schemes suffer from computational noise and instability issues. The proposed method is advantageous as it does not require temporal discretization for the solution of the ADEs as well as it does not suffer from numerical instability. The reliability and effectiveness of the presented algorithm is investigated by sufficient large number of independent runs and comparison of results with other existing numerical methods. The results show that the present method removes the difficulties arising in the solution of the ADEs and provides solution with good accuracy.

1. Introduction

The ADE has been widely used to describe the movement of contaminants in the subsurface. It is a challenging problem in engineering and environmental sciences, and a problem of great importance to understand the transportation of chemical or biological contaminants through subsurface aquifer systems [1,2]. The fate and transport of solutes in soils and groundwater have been a focus of experimental and theoretical research in subsurface hydrology. In many practical situations, one needs to predict the time behavior of a contaminated ground water layer. ADE has also been used to describe heat transfer in draining film [3], flow in porous media [4], mass transfer [5], water transports in soils [6], pollutant transport in rivers and streams [7,8], dispersion of dissolved material in estuaries and coastal seas [9,10], and thermal pollution in river

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system [11]. The numerical solution of ADE plays an important role in providing approximate estimates of contaminant concentration distributions in soils or aquifer systems. A number of analytical solutions have been developed for one-, two-, or three-dimensional ADE. In three dimensions, ADE is given by:

$$\frac{\partial c}{\partial t} + A_x \frac{\partial c}{\partial x} + A_y \frac{\partial c}{\partial y} + A_z \frac{\partial c}{\partial z} = B_x \frac{\partial^2 c}{\partial x^2} + B_y \frac{\partial^2 c}{\partial y^2} + B_z \frac{\partial^2 c}{\partial z^2} \tag{1}$$

where A_x, A_y, and A_z are the velocity components of advection in the direction x, y and z, respectively, whereas B_x, B_y, and B_z are the dispersions in the—x, y, and z, directions respectively.
In this article we consider the unsteady one-dimensional ADE defined by:

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} = B \frac{\partial^2 c}{\partial x^2} \tag{2}$$

where $0 \le x \le 1$ and $0 < t \le T$, together with the following initial and BCs:

$$c(x,t) = \begin{cases} f(x), & \text{at } t = 0,\ 0 \le x \le 1 \\ g_0(t), & \text{at } x = 0,\ 0 < t \le T \\ g_1(t), & \text{at } x = 1,\ 0 < t \le T. \end{cases} \tag{3}$$

The literature contains many methods for solving ADE of one-, two-, or three-dimensional problems. Van Genuchten and Alves [12] calculated analytical solutions for the one-dimensional ADE subject to various initial and BCs. Analytical solutions for two- and three-dimensional ADE have been presented by Batu [13] and Leij et al. [14], respectively. Numerical schemes, such as the alternating group explicit (AGE) method, higher order alternating direction implicit (ADI) method, exponential compact difference (ECD) scheme, and finite difference method (FDM) have been presented by various authors [15–19] for the numerical solution of ADE. A significant amount of work has been dedicated to the development of the FDM and its various finite difference schemes [20–23] for the solution of ADE. The accuracy of the difference schemes constructed using most of the above methods was second order in time and fourth order in space. Therefore, a higher order exponential (HOE) scheme was developed by Tian and Yu [24] to achieve higher order accuracy in both the space and temporal components. Several variations of the ADI methods have been also developed for the solution of two-dimensional ADEs [16,25]. In Ref. [26], the finite element method (FEM) was used by Huang et al. for the solution of the fractional ADE. Recently, a comparison of three numerical schemes: the third order upwind explicit scheme (UES), the fourth order UES and the nonstandard finite difference (NSFD) scheme of FDM was performed by Appadu et al. [27]. All the above methods for solving ADE require spatial as well as temporal discretization and the accuracy of the solution depends upon some optimal value of the spatial step sizes. In addition, some of the methods become unstable for higher values of the Peclet number and show nonphysical oscillations.

Due to the complexity of solving ADE using traditional numerical methods, we present a method based on neural networks for the solution of the unsteady ADEs with different parameter values. It has been already shown in the literature that ANN methods are capable of solving ordinary differential equations (ODEs) as well as partial differential equations (PDEs) arising in real world applications [28–31]. The ANN method has come up as an alternative for the approximate solution of differential equations (DEs) as it avoids the deficiencies associated with the existing numerical methods in the literature. For instance, traditional numerical methods require domain discretization and special treatment is imperative for nonlinear DEs, but the ANN method does not require any special treatments and is more general. A survey article [32] in 2011 presented roughly 50 studies on ANN methods for the solution of DEs. The length factor ANN method, proposed by McFall et al. [33,34] for solving DEs is found to be more powerful and unique among other ANN methods for solving DEs with arbitrary BCs. Thus, in this paper we use the length factor ANN method for the numerical solution of ADE with defined initial or BCs.

The rest of the paper is organized as follows: Section 2 presents the dimensionless form of ADE. An introduction to the ANN method for solving ADE is presented in Section 3. Section 4 then explains the test problems along with their formulation and numerical simulation results. The calculation of errors and the comparison with other numerical methods are presented in Section 5. Finally Section 6 contains the conclusion of the paper.

2. Advection–dispersion equation

The advection–dispersion is one of the most important models of mathematical physics and it describes the advection and dispersion of mass, heat, energy, velocity, vorticity, etc. Mathematically, the classical ADE can be written as [35]

$$\frac{\partial c}{\partial \tau} = -\upsilon \frac{\partial c}{\partial \xi} + d \frac{\partial^2 c}{\partial \xi^2}, \quad \xi \in (0, L), \tau > 0 \tag{4}$$

subject to the BCs

$$c(\xi, 0) = 0, \qquad c(0, \tau) = c_0, \qquad c(L, \tau) = 0,$$