

Numerical solution of non-linear advection-dispersion equation in a finite porous domain

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Abstract

This study presents a numerical simulation of the one-dimensional concentration-dependent convection-dispersion equation in a finite heterogeneous porous formation. The solution of the convection-diffusion equation with variable coefficients is obtained with the help of MATLAB pdepe solver. The groundwater flow velocity depends on the pollutant concentration, and the dispersion coefficient is proportional to the groundwater flow velocity. The effects of the zero-order production term and the first-order decay are also considered. The aquifer is assumed to be heterogeneous and finite, with sources concentrated in the flow direction. It is assumed that the porous media and the pollutant are chemically non-reactive. Initially porous domain is considered not solute free. The model assumes a uniform continuous input point source and a variable input point source released from the left end of the aquifer domain. The obtained results graphically describe the importance of the dispersion coefficient and other relevant parameters for solute transport in porous media. The developed numerical solution is verified with an analytical solution, and it is found that they are in good agreement.

Keywords: Advection, dispersion, uniform and varying input, non-linear equation, pdepe solver

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1. Introduction

Groundwater resources have recently suffered catastrophic damage due to the seepage of industrial and agricultural pollutants into the subsurface. Therefore, it is very important to pay attention to the protection of groundwater resources. Nowadays, researchers are very concerned about the adverse effects of poor groundwater quality on human health and ecosystems. Groundwater pollution may vary from place to place. Estimating the concentration of contaminants in groundwater systems is critical to minimizing the risk and vulnerability of aquifers. Soil type, porosity, hydraulic conductivity, specific yield, etc. are all important factors affecting how an aquifer degrades during solute transport. The main factors that significantly affect the movement of solutes in porous media are dispersion, velocity and the type of contaminants. In groundwater systems, solute transport is typically modeled using linear/non-linear advection-dispersion equation (ADE), which can add equilibrium absorption and first-order decay. Mathematical models play an important role in assessing their effects correctly. Numerous mathematical studies using point and non-point sources have been performed to determine the concentrations of pollutants in aquifer systems (Yadav et al., 1990, Kumar and Yadav, 2015, Singh and Chatterjee, 2016). Van Genuchten (1980) derived an analytical solution

for chemical transport with zero-order production and first-order decay. Batu (1982) developed two-dimensional time-dependent infiltration and evaporation of non-uniform and non-periodic band sources in homogeneous porous media.

Analytical solutions to mathematical models explaining pollution movements are nearly impossible if significant hydraulic and chemical processes are considered simultaneously (Massaboo et al., 2006). Analytical solutions to convection-diffusion equations are usually restricted to one-dimensional problems, including growth and decay terms for semi-infinite or infinite domains. Dhawan et al., (2012) proposed a numerical solution to the convection-diffusion problem using explicit and implicit finite-difference approximations. Singh and Das (2015) presented the scale dependent solute dispersion with linear isotherm in heterogeneous medium. Liu and Wang, (2015) studied the higher-order numerical solutions of the convection-diffusion equations in a different approach. In finite porous media, Jaiswal and Yadav (2014) developed an analytical solution for the transport of pollutant with a uniform flow velocity under a pulse type input source, while Singh et al., (2015) developed an analytical solution for solute transport with sinusoidal varying velocities with a pulse-type point source. Andallah and Khatoon, (2020) developed numerical solutions to the convection-diffusion equations using finite-difference schemes. For variable input point sources in semi-infinite porous medium, Yadav and Kumar (2021) developed an analytical solution for conservative solute transport in 2D. Kumar, et al., (2022) obtained the numerical solution of one dimensional advection-dispersion equation with uniform and varying boundary conditions for heterogeneous porous medium. When the velocity and dispersion fields are complex and time-varying, the transport process cannot be estimated analytically, instead, numerical approximations are required. To provide an estimate of the distribution of pollutant concentrations in a soil or aquifer system, the numerical solution of ADE is important.

In this paper, a numerical solution to a one-dimensional non-linear advection-diffusion equation is obtained using the MATLAB pdepe script. Contaminants are chemically non-reactive, and porous media is heterogeneous and finite in length. Hydrodynamic dispersion and groundwater velocity depends on solute concentration and is considered to be decreasing in nature. We also consider the zero-order production and the first-order decay terms. The medium is supposed to be finite, horizontally long, and heterogeneous. Numerical solutions are obtained for both uniform and varying types of input point sources. The porous domain initially contains some solute concentration, i.e., at first the medium is not solute-free. At the left end of the domain ($x = 0$), a point source is introduced, and at the right end of the domain, a second boundary condition (flux type) is applied. A set of hydrological input data taken from published research articles are used to provide a graphical representation of the concentration distribution.

2. Mathematical formulation of the Problem

Consider a one-dimensional heterogeneous porous domain of finite length, measured from its source in which solute transport occurs from the left end to the right. Groundwater flow is assumed to be along the longitudinal direction, as shown in the schematic diagram (Figure 1). The aquifer is continuously injected with a constant amount of solute c_0 at the end ($x = L_1$). The maximum concentration decreases with the position as a result of groundwater convection, which transfers and disperses the mass of the solute during the process.

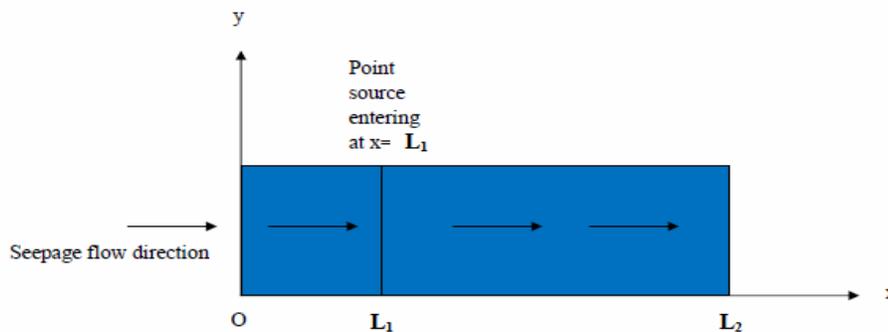


Figure 1: Schematic view of the proposed problem

The convection-diffusion equation of groundwater pollution is essentially an expression of mass conservation, which is expressed by a second-order partial differential equation as follows (Freeze and Cherry, 1979 and Bear, 1972).

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D(x, t) \frac{\partial c}{\partial x} - u(x, t) c \right) - \gamma c + \mu \tag{1}$$

where $c[ML^{-3}]$ is the solute concentration in the liquid phase. $x[L]$, $t[T]$ are space and time variable, respectively. $D[L^2T^{-1}]$ is the solute dispersion coefficient. $u[LT^{-1}]$ is the velocity of the flow. D and u may be constants or functions of a single variable or a set of variables, such as time, space, concentration, etc. Solute particles diffuse from their initial positions when there

is velocity at the pore scale. The dispersion coefficient D on the Darcy scale describes the spreading process. $\gamma[T^{-1}]$ is first order decay rate coefficients and $\mu[ML^{-3}T^{-1}]$ is zero-order production. Depending on the value of the dispersion coefficient, the Eq. (1) becomes parabolic or hyperbolic. Numerical solutions of partial differential equations have proven challenging, especially when modeling nonlinear advection-diffusion equations.

Hydraulic gradients vary in time and space, causing velocities to vary in time and space. The behavior of groundwater depends on whether hydraulic conductivity is significantly reduced or increased. It is assumed that the dispersion coefficient and groundwater velocity are both concentration-dependent functions:

$$\left. \begin{aligned} u(x,t) &= u_0 f(bc) \\ D(x,t) &\propto u \Rightarrow D(x,t) = D_0 f(bc) \\ \gamma(x,t) &= \gamma_0 f(bc) \\ \mu(x,t) &= \mu_0 f(bc) \end{aligned} \right\} \quad (2)$$

Here, $b[M^{-1}L^3]$ represents a parameter whose dimension is inversely proportional to the solute concentration. So, $f(bc)$ is a dimensionless expression. It is also assumed that $f(bc)$ is bounded and $f(bc)=1$ at $b=0$ or $c=0$. If $(b=0)$, it means uniform constant flow, on the other hand, if $(c=0)$, it means that there is no solute in the medium. Where $f(bc)$ is an arbitrary function that depends on the solute concentration under the above conditions, however in order to discuss the mathematical model, we simply take into account the following two categories of functions:

$$\left. \begin{aligned} (i) \quad & f(bc) = \exp(-bc) \\ (ii) \quad & f(bc) = |1 + \sin(bc)| \end{aligned} \right\} \quad (3)$$

2.1 Input Condition of Uniform Nature

The pollutant is assumed to be inert, there are no additional sinks or points downstream of the source, and the vertical and lateral components of the flow velocity are assumed to be zero. The model simulates the concentration along a one-dimensional flow in a finite heterogeneous porous medium, where the groundwater flow is considered to be along the longitudinal direction, i.e. the x -axis (from $x=L_1$ to $x=L_2$). Initially, the porous domain is not solute-free, meaning that there is some concentration in the domain before solute injection. A uniform constant input source enters from the left end of the porous domain. Large quantities of solutes are carried by groundwater flow, during which slugs of solutes diffuse, resulting in a decrease in maximum concentration with position. In order to solve Eq.(1) we imposed the following initial and boundary conditions as follows:

$$c(x,t) = c_i \exp(-ax) \quad ; \quad t=0, \quad L_1 \leq x \leq L_2 \quad (4)$$

$$c(x,t) = c_0 \quad ; \quad t > 0, \quad x = L_1 \quad (5)$$

$$\frac{\partial c(x,t)}{\partial x} = 0 \quad ; \quad t \geq 0, \quad x = L_2 \quad (6)$$

where u_0, D_0, γ_0 and μ_0 denote initial constant of velocity, dispersion coefficient, first order decay and zero order production, respectively.

Substituting Eq.(2) into Eq. (1, 4-6), we have

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D_0 f(bc) \frac{\partial c}{\partial x} - u_0 f(bc) c \right) - (\gamma_0 c - \mu_0) f(bc) \quad (7)$$

Initial and boundary conditions are

$$c(x,t) = c_i \exp(-ax) \quad ; \quad t=0, \quad L_1 \leq x \leq L_2 \quad (8)$$

$$c(x,y) = c_0 \quad ; \quad t > 0, \quad x = L_1 \quad (9)$$

$$\frac{\partial c(x,t)}{\partial x} = 0 \quad ; \quad t \geq 0, \quad x = L_2 \quad (10)$$

2.2 Input Condition of Varying Nature

The input condition given by Eq.(9) implies that the input concentration at the entry of the medium remains the same at all times but this is not always possible in practice. Input concentrations at the source may vary over time due to various human activities. This situation is mathematically represented by the mixed condition. The source of input concentration may vary with time due to variety of reasons. The variation in pollution level is mainly attributable to the intrusion of municipal and industrial sewage into groundwater basins. One way to represent such a condition is to consider a factor on the right hand side of the input condition Eq.(9), where $g(mt)=1$ for $m=0$ or $t=0$. The first case ($m=0$) represents the steady flow and second case ($t=0$) represents the initial state.

Here m denotes an unsteady parameter whose dimension is inversely proportional to the time variable. Hence, $g(mt)$ is a non-dimensional expression. In the proposed problem, a numerical solution is developed for the sinusoidal form of the time-varying input i.e. $g(mt) = 1 + \sin(mt)$. This situation can be described mathematically by the following mixed-type or third-type condition:

$$-D \frac{\partial c(x,t)}{\partial x} + u c(x,t) = u_0 c_0 \{1 + \sin(mt)\} \quad ; \quad t > 0, \quad x = L_1 \tag{11}$$

Substituting Eq. (2) into Eq. (11) we have

$$-D_0 f(bc) \frac{\partial c(x,t)}{\partial x} + u_0 f(bc) c(x,t) = u_0 c_0 \{1 + \sin(mt)\} \quad ; \quad t > 0, \quad x = L_1 \tag{12}$$

Now using input condition Eq. (12) in place of Eq. (9), we obtain the numerical solution for varying input point source. Other conditions are same as in uniform input source.

3. Numerical Solution of the Proposed Problem

To demonstrate the concentration distributions for two different input sources, (uniform and varying nature) numerical solutions of the governing Eq.(1) are displayed graphically using hydrological input data. In both cases, the aquifer domain is assumed to be finite and heterogeneous, and the decay of concentration over space and time is examined for different hydrological parameter values. Numerical solutions are obtained using MATLAB pdepe solver, and the concentration behavior is displayed graphically. The common input data taken in this paper are chosen from previous published literature or empirical relationship. There is no doubt that the groundwater flow velocity usually varies between 2 (meter/day) and 2 (meter/year), depending on the geological formation (Todd, 1980). Concentration values are evaluated with reference concentrations as: $c_0 = 1.0, c_i = 0.01$. The units of distance and time are in meter and day, respectively. The common input data are taken as initial groundwater velocity $u_0 = 0.12$ (meter/day), initial dispersion coefficient $D_0 = 0.20$ (meter²/day), heterogeneous parameter $a = 0.015$ (meter⁻¹), unsteady parameter $m = 0.01$ (day⁻¹), $b = 0.1$ (meter³/kg), initial first order decay $\gamma_0 = 0.0020$ (day)⁻¹, and initial zero order production $\mu_0 = 0.0025$ (kg/meter³ day), time $t = 4$ (day). The range of finite domain is from $L_1 = 0$ to $L_2 = 5$ (meter). Graphical representations of the solute concentration scenario in the aquifer domain with different physical parameters are shown.

3.1 Case-I: For a uniform input point source, the concentration distributions are shown by surface and line graphs in Figures (2-3) and (4-5), respectively.

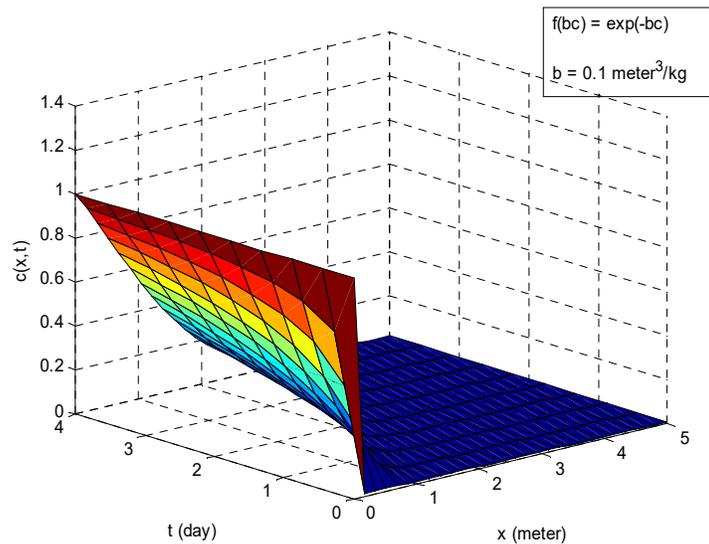


Figure 2: Dimensionless solute concentration distributions for exponential decreasing nature for Eq. (7) in uniform continuous type input point source.

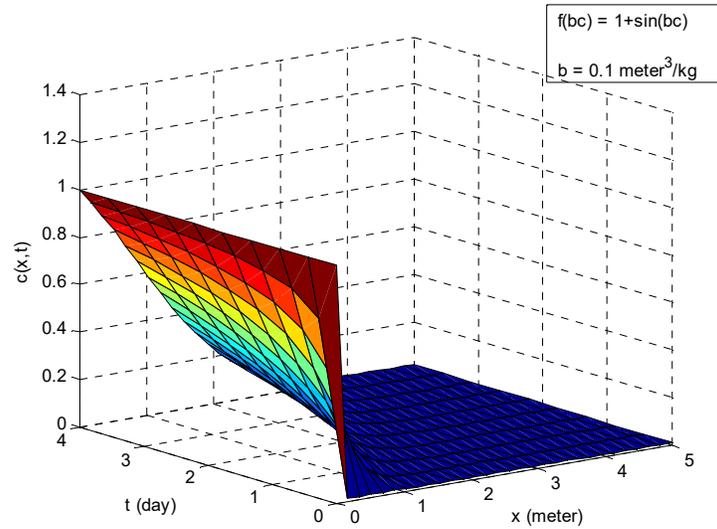


Figure 3: Dimensionless solute concentration distributions for sinusoidal nature for Eq. (7) in uniform continuous type input point source

Figures (2, 3) describe the dimensionless concentration distribution predicted for a uniform input point source by the numerical solution of Eq. (7) for exponential decreasing and sinusoidal nature velocity, respectively. In both graphs, the concentration level is decreasing with time and position. The concentration pattern decreases more rapidly than the position with respect to time, and beyond a predetermined distance, it becomes constant in both time and space. The exponential decreasing nature has a somewhat faster tendency to decrease than the sinusoidal nature.

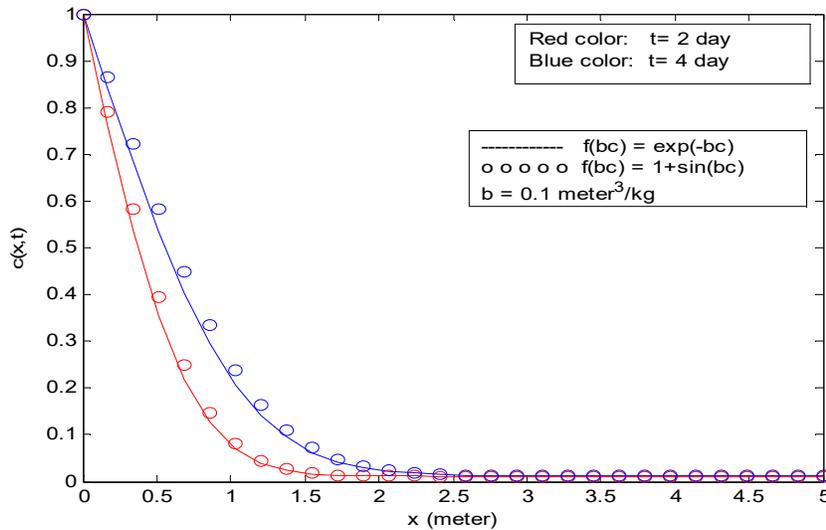


Figure 4: Comparison of dimensionless solute concentration distributions for Eq. (7) at different time in uniform continuous type input point source.

The distribution of the concentration profiles predicted by Eq.(7) for a uniform continuous input point source is shown in Figure (4) at two different time. At any given location, the concentration level is higher for a longer period, lower for a lower time, and stabilizes by reaching the other end of the domain. Furthermore, the exponential decreasing function has a slightly faster concentration attenuation compared to the sinusoidal function. It is clear from the figure that for a uniform input point source, the initial concentration levels are the same at both time.

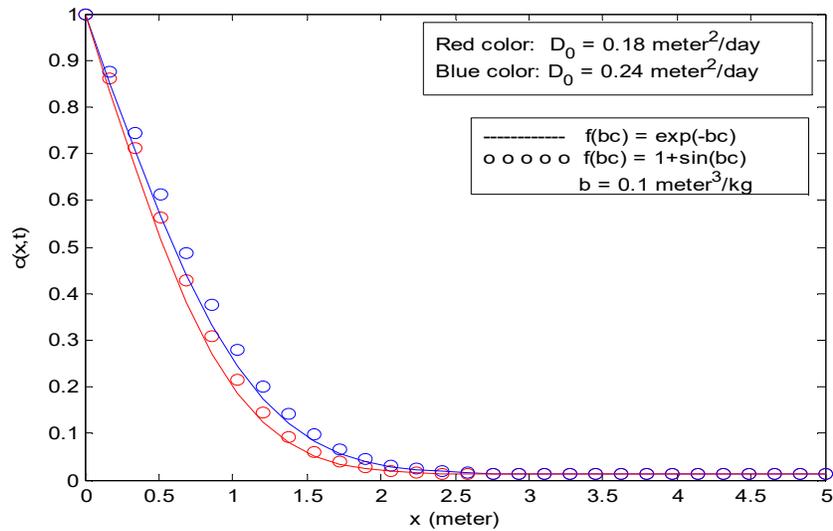


Figure 5: Comparison of dimensionless solute concentration distributions for Eq. (7) at different dispersion coefficient in uniform continuous type input point source at $t = 4$ day.

Figure (5) shows the concentration distribution for uniform continuous input point source for two different dispersion coefficients, with the other parameter remaining unchanged at $t = 4$ day . At a specific location in the domain, the concentration level is lower with a lower value of dispersion coefficient and higher with a higher value of dispersion coefficient. Furthermore, it is worth noting that the exponentially decreasing function exhibits a slightly faster rate of concentration decay than the sinusoidal function. The concentration pattern increases with dispersion coefficient and decreases with space, and after a certain distance it remains constant in all time and space.

3.2 Case-II: Figures (6-7) and (8-9) represent the concentration distributions by surface and line graphs for varying input point source.

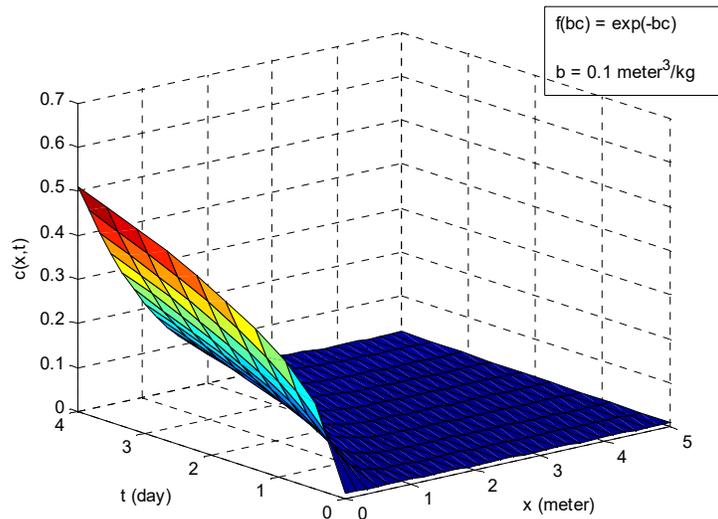


Figure 6: Dimensionless solute concentration distributions for exponential decreasing nature for Eq. (7) in varying nature input point source.

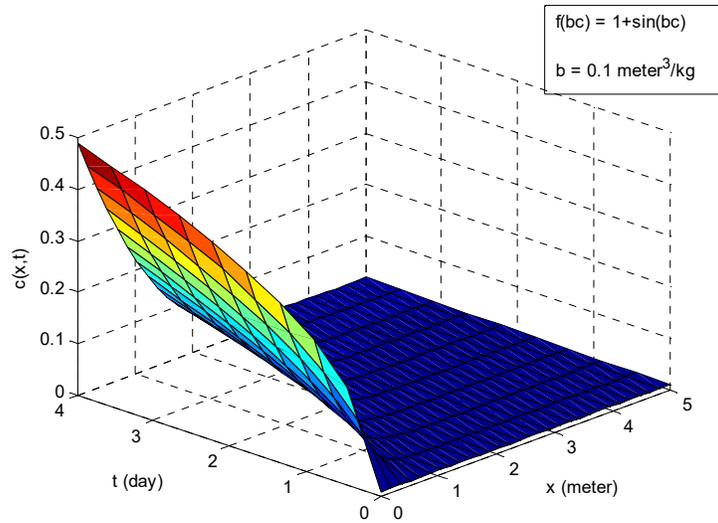


Figure 7: Dimensionless solute concentration distributions for sinusoidal nature for Eq. (7) in varying nature input point source.

For varying input point source, the dimensionless concentration distributions estimated numerically with 300 grid points are shown in Figures (6) and (7) for exponentially decreasing and sinusoidal nature velocity, respectively. The concentration pattern drops faster with respect to time than position, and over a predetermined distance, it becomes a relative constant in time and space. In both graphs, a downward trend in concentration distribution with position and time is noted for both exponentially decreasing and sinusoidal natures.

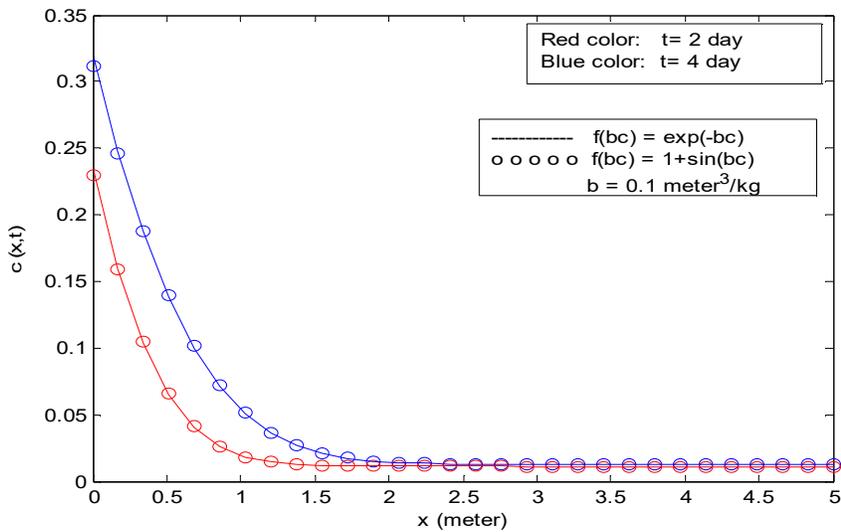


Figure 8: Comparison of dimensionless solute concentration distributions for Eq. (7) at different time in varying nature input point source.

The concentration profiles evaluated by Eq. (7) at two different times for varying nature input point sources are shown in Figure (8). The level of attention varies with space and time, while it is always decreasing; it is noticed lower in lower periods of time and higher in longer periods of time. Furthermore, the concentration attenuation is almost the similar for both types (exponentially decreasing and sinusoidal nature). After some distance from the origin, the concentration pattern stabilizes. Due to the varying nature of the input point source, it can be noticed that the initial concentration level varies with time.

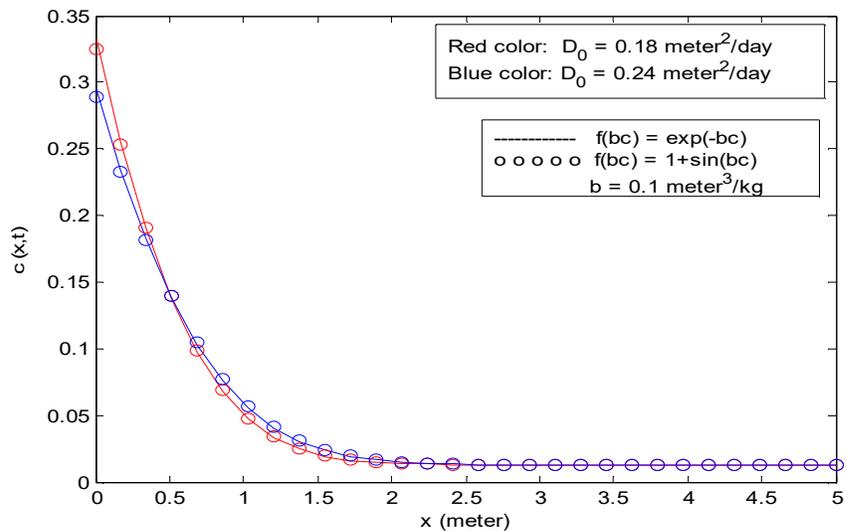


Figure 9: Comparison of dimensionless solute concentration distributions for Eq. (7) at two different dispersion coefficients in varying nature input point source at $t = 4$ day .

The concentration distribution is shown in Figure (9) for two different dispersion coefficient for input point source of various properties, keeping other parameters the same as the previous one at $t = 4$ day . A higher dispersion coefficient corresponds to a lower concentration level, and a lower dispersion coefficient corresponds to a higher concentration level near the source boundary. However, when one moves away from the source boundary, this pattern reverses due to the different nature of the input sources. In both cases (sinusoidal and exponentially decreasing properties), the concentration decay is nearly identical. After traveling a certain distance from the inlet boundary, the concentration pattern becomes constant, although it decreases with respect to space and increases with respect to the dispersion coefficient.

4. Validation of Numerical Solution

Numerical solutions were developed under the assumption that both groundwater velocity and dispersion coefficient depend on concentration. Hence, it is difficult to find an analytical solution to this problem. We convert this mathematical model from variable coefficients to constant coefficients in order to validate the numerical solution. For this, we use the following values in Eq.(2) and Eq.(3), as: $b = 0, a = 0, m = 0, \gamma = 0$ and $\mu = 0$, we have

$$u(x,t) = u_0 \quad \text{and} \quad D(x,t) = D_0 \tag{13}$$

Substituting the values from Eq.(13) into Eq. (1 and 4-6) we have;

$$\frac{\partial c}{\partial t} = D_0 \frac{\partial^2 c}{\partial x^2} - u_0 \frac{\partial c}{\partial x} \tag{14}$$

Initial and boundary conditions for uniform type input point source for the finite domain $L_1 = 0$ to $L_2 = l$ are given by;

$$c(x,t) = c_i \quad ; \quad t = 0 \quad , \quad 0 \leq x \leq l \tag{15}$$

$$c(x,t) = c_0 \quad ; \quad t > 0 \quad , \quad x = 0 \tag{16}$$

$$\frac{\partial c(x,t)}{\partial x} = 0 \quad ; \quad t \geq 0 \quad , \quad x = l \tag{17}$$

Now the initial and boundary value problem Eqs. (14-17) in the (x,t) domain becomes similar to that of Cleary and Adrian (1973) in the (x,t) , quoted as problem A3 (van Genuchten and Alves, 1982), hence or else using the Laplace integral transform technique, the desired analytical solution can be written as follows:

$$c(x,t) = c_i + (c_0 - c_i) A(x,t) \tag{18}$$

where,

$$A(x,t) = \frac{1}{2} \operatorname{erfc} \left[\frac{x-u_0t}{2\sqrt{D_0t}} \right] + \frac{1}{2} \exp \left[\frac{u_0x}{D_0} \right] \operatorname{erfc} \left[\frac{x+u_0t}{2\sqrt{D_0t}} \right] + \frac{1}{2} \left\{ 2 + \frac{u_0(2l-x)}{D_0} + \frac{u_0^2t}{D_0} \right\} \exp \left[\frac{u_0l}{D_0} \right] \operatorname{erfc} \left[\frac{2l-x+u_0t}{2\sqrt{D_0t}} \right] - \sqrt{\frac{u_0^2t}{\pi D_0}} \exp \left[\frac{u_0l}{D_0} - \frac{(2l-x+u_0t)^2}{4D_0t} \right]$$

The boundary conditions for varying nature of input point source may be expressed as:

$$-D_0 \frac{\partial c(x,t)}{\partial x} + u_0 c(x,t) = u_0 c_0 \quad ; \quad t > 0, \quad x = 0 \quad (19)$$

Advection-dispersion equation Eq. (14), as well as the initial condition Eq. (15), the input condition Eq. (19), and the second boundary condition Eq. (17) constitute a problem in a domain (x,t) that is comparable to Bastian and Lapidus (1956) and Brenner (1962) quoted as the problem A4 (van Genuchten and Alves 1982). Therefore, using the Laplace integral transform technique, the required analytical solution can be written as follows:

$$c(x,t) = c_i + (c_0 - c_i) \{P(x,t) + Q(x,t)\} \quad (20)$$

where,

$$P(x,t) = \frac{1}{2} \operatorname{erfc} \left[\frac{x-u_0t}{2\sqrt{D_0t}} \right] + \sqrt{\frac{u_0^2t}{\pi D_0}} \exp \left[-\frac{(x-u_0t)^2}{4D_0t} \right] - \frac{1}{2} \left\{ 1 + \frac{u_0x}{D_0} + \frac{u_0^2t}{D_0} \right\} \exp \left[\frac{u_0x}{D_0} \right] \operatorname{erfc} \left[\frac{x+u_0t}{2\sqrt{D_0t}} \right]$$

$$Q(x,t) = \sqrt{\frac{4u_0^2t}{\pi D_0}} \left\{ 1 + \frac{u_0(2l-x+u_0t)}{4D_0} \right\} \exp \left[\frac{u_0l}{D_0} - \frac{(2l-x+u_0t)^2}{4D_0t} \right] - \frac{u_0}{D_0} \left\{ 2l-x + \frac{3u_0t}{2} + \frac{u_0(2l-x+u_0t)^2}{4D_0} \right\} \exp \left[\frac{u_0l}{D_0} \right] \operatorname{erfc} \left[\frac{2l-x+u_0t}{2\sqrt{D_0t}} \right]$$

We now compare the analytical solutions obtained in Eq.(18) and Eq.(20) with the numerical solutions developed by the MATLAB pdepe script for input point sources of uniform and variable nature, respectively with the help of graphs.

The comparison between the analytical solution Eq. (18) of the convection-diffusion equation with constant coefficients obtained by the Laplace integral transform technique and the numerical solution Eq. (14) obtained by the MATLAB pdepe script is shown in Figure (10). With all other parameters held constant, both analytical and numerical solutions can be obtained for the dimensionless concentration distribution of the uniform continuous input point source at two different times. The solute concentration declines over time and space, as shown in Figure (10), until becoming constant at a given distance. Both the analytical and the numerical solutions concentration distribution patterns accord well.

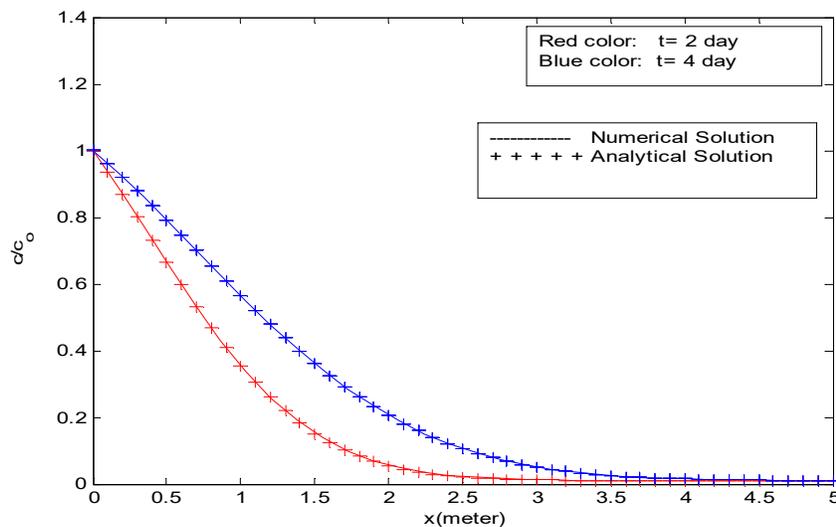


Figure 10: Comparison of concentration distributions for analytical solution in Eq. (18) and numerical solution of Eq. (14) for uniform continuous input point source.

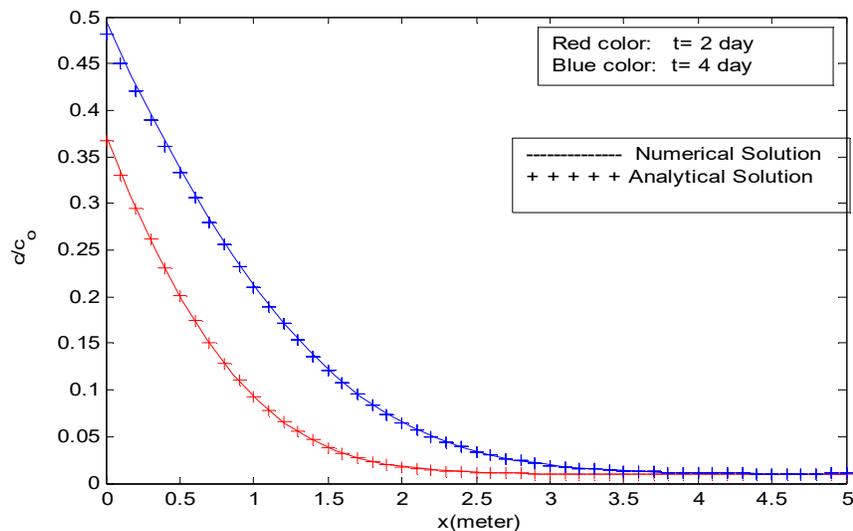


Figure 11: Comparison of concentration distributions for analytical solution in Eq. (20) and numerical solution of Eq. (14) for varying nature input point source.

Figure (11) represents the dimensionless concentration distribution of the analytical solutions of Eq. (20) and numerical solution Eq. (14) obtained by the MATLAB pdepe script for two different times. Input source is assumed varying nature and the common input values are taken as $u_0 = 0.12$ (meter/day), $D_0 = 0.20$ (meter²/day), $t = 4$ (day). The range of finite domain is from $L_1 = 0$ to $L_2 = 5$ (meter). The concentration patterns for both analytical and numerical solutions are notably similar, diminish with time and space, and then become constant throughout domain after a given distance.

As can be seen from Figures (10) and (11), the solutions generated using the numerical method MATLAB pdepe solver are valid for both uniform and variable type input point source conditions. Such solutions would be very useful for the more general dispersion problem in a finite field. The solute concentration dependence of solutions with all possible combinations is compared graphically. Based on this, we can say that our numerical solution to the nonlinear problem is almost the best of my knowledge. Also, the analytical solution obtained with help of Laplace integral transform technique is similar to one obtained by Kumar et al. (2009). LITT is simpler, more viable and commonly used in assessing the stability of numerical solutions in more realistic dispersion problems, to understand and manage the pollution distributions along groundwater, surface water and air flow domains.

4. Conclusions

For one-dimensional finite, heterogeneous porous media, a numerical solution to the advection-dispersion equation for a uniform constant and variable input point source is found using the MATLAB pdepe script. It is vital to evaluate the sustainability of such realistic numerical solutions in order to comprehend, evaluate, and manage the effects of groundwater, surface water, and air pollution. The numerically generated solutions are contrasted with a known published analytical solution in the current work. These solutions would be very beneficial for nonlinear convection-dispersion equation problems. The results of this study emphasize the importance of dispersion function and solute retention in a heterogeneous finite porous medium. The analysis of the results shows that when the value of the dispersion function is high, the concentration distribution decreases rapidly. Graphs are used to compare solutions for all possible combinations of different parameters. This work considers the dependence of the convective-dispersive term, the transient velocity, the first-order decay, and the zero-order production on the solute concentration. The numerical solutions of the nonlinear advection-diffusion equation are useful to assess the time and position at which the concentration level of the pollutants will start affecting polluted water and eco-system. Determining the level of contaminated water in an aquifer system and outlining possible measures is the goal of this work.

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