Modeling of the transport and fate of radioactive constituent in groundwater

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Abstract

This paper introduces a methodology for developing a numerical scheme for the solution of the advection dispersion process in ground water. The study necessitates the solution of the differential equation describing the solute transport process hereafter referred to as the dispersion equation. A straightforward analytical solution for the most general form of this equation is not known to this date. Most of the available analytical solution for dispersion problems is of simplified cases or simple boundary conditions etc. Complexities of the problem cannot be well addressed with the analytical solution and hence there is a necessity to develop numerical models. A numerical solution of the governing equation using Finite Difference Method has been attempted in this study. Based on the proposed methodology three different cases of upstream boundary condition for a radioactive pollutant is considered. Results of the proposed scheme are compared with the analytical solution of the advection dispersion equation. Proposed scheme accurately simulates the concentration – distance profile of the cases under consideration.

1 Introduction

A variety of chemical and radioactive constituents get transported by water in surface as well as ground water. Their presence in small quantities may result in environmental hazards/disaster and is of concern to environmental and hydraulic engineers. Their accurate prediction is very crucial to plan for the effective
environmental management and remedial measures. Reynolds's transport theorem can be used to arrive at governing equation of mass, momentum and energy conservation of different physico-chemical kinetics and other process. For most of the environmental applications wherein mass of the constituent is negligible as compared to the mass of water, the momentum, potential energy and kinetic energy of constituent have negligible effect in their transport. Hence mass conservation equation also called as advection-diffusion equation is often adequate and is used for almost all applications.

Analytical solutions of transport equation for different cases are available in literature (Marino [4]). Almost all-available analytical solutions are restricted to simple initial and boundary conditions, coefficients with unrealistically simple functions of space and/or time, uniform flow, and thereby have a limited practical relevance. Apart from these limitations, the implementation of these analytical solutions often require numerical evaluation of complex convolution integrals (Bennett [1]), which are computationally expensive as compared to numerical solutions of transport equations. Further, due to numerical evaluation of these integrals, the accuracy of analytical solutions can no longer be claimed to be superior to numerical schemes. Hence, for most of the practical applications that involves complex initial and boundary conditions, modelers are forced to resort to the numerical solution of transport equations. For the present study Holly-Preissman scheme is used for numerical solution of advection equation and an explicit finite difference scheme is used for diffusion term.

2 One-dimensional transport equation for ground water

The general one-dimensional transport equation can be written as,

$$\frac{\partial (AC)}{\partial t} + \frac{\partial (AUc)}{\partial x} = \frac{\partial}{\partial x} \left( ADL \frac{\partial c}{\partial x} \right)$$

(1)

Where,

\[ u = \text{Longitudinal velocity} \]
\[ A = \text{Cross sectional area} \]
\[ DL = \text{Longitudinal dispersion coefficient} \]

Assuming cross-sectional area 'A', and longitudinal velocity 'U= u' a constant, the equation can be simplified as,

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = DL \frac{\partial^2 c}{\partial x^2}$$

(2)
3 Initial condition

The solution of advection-diffusion equation requires specification of initial concentration $c$ at time $t = 0$ for all grid points. In case of conservative and non-conservative pollutant, initial concentration of the pollutant is to be specified as initial condition. Depending upon the types of applications, the initial conditions may change. For present study three different cases are studied. The initial condition for all the three case is $c(x, 0) = 0$ units.

4 Boundary conditions

Apart from initial condition, for the solutions of advection-diffusion equations, two boundary conditions are required, one at the upstream end, and other at the downstream end.

4.1 Upstream boundary condition

The upstream boundary condition is defined in terms of a fixed concentration at the upstream boundary. This boundary condition represents the solute concentration entering the system. For solutions of the unsteady / time variant equations a pollutograph is used as the upstream boundary condition. Upstream boundary condition also depends on types of application dealt. The upstream boundary conditions for the three cases are

i) Case I: $c(0,t) = c_0$ 
(t>0)

ii) Case II: $c(0,t) = c_0 e^{\lambda t}$
(t>0)

iii) Case III: $c(0,t) = c_0 (1-e^{-\lambda t})$
(t>0)

Where $c_0$ is the input concentration and $\lambda$ is a decay coefficient.

4.2 Downstream boundary condition

Like upstream boundary a time varying solute concentration or a pollutograph can also be specified as down stream boundary condition. However, in the absence of these, often a specified dispersive flux usually set to zero ($\partial C/\partial x = 0$), is used as downstream boundary condition. (Cunge et al. 1980).

5 Analytical solution

The case of one-dimensional dispersion in ground water has been studied with a view to compare the finite difference method results with those of analytical solution. This has been possible mainly due to the fact that the closed form analytical solutions are available for one-dimensional dispersion equation. For the study of one-dimensional dispersion, the following three cases of upstream
boundary conditions specifying the input concentrations were considered (Pygude [6]).

i) Case I: \( c(0,t) = c_0 \)  
\( \quad (t > 0) \)

ii) Case II: \( c(0,t) = c_0 e^{\lambda t} \)  
\( \quad (t > 0) \)

iii) Case III: \( c(0,t) = c_0 (1-e^{-\lambda t}) \)  
\( \quad (t > 0) \)

Where \( c_0 \) is the input concentration and \( \lambda \) is a coefficient.

Marino [4] has given the analytical solution to the one-dimensional dispersion equation for each of the above cases of the upstream boundary conditions. The solutions according to Marino [4] are given below:

i) Case I

\[
c(x,t) = \frac{C_0}{2} \left\{ \text{erfc} \left( \frac{x-ut}{2\sqrt{D_L t}} \right) + \exp \left( \frac{ux}{t} \right) \text{erfc} \left( \frac{x+ut}{2\sqrt{D_L t}} \right) \right\}
\]

ii) Case II

\[
c(x,t) = \frac{C_0}{2} \exp(\gamma t) \left\{ \exp \left[ \frac{x(u - \phi)}{2D} \right] \text{erfc} \left( \frac{x - \phi t}{2\sqrt{D t}} \right) + \exp \left[ \frac{x(u + \phi)}{2D} \right] \text{erfc} \left( \frac{x + \phi t}{2\sqrt{D t}} \right) \right\}
\]

where,

\( \phi = (u^2 + 4\gamma D)^{1/2} \)

iii) Case III

\[
c(x,t) = \frac{1}{2} \left\{ \text{erfc} \left( \frac{x-ut}{2\sqrt{D t}} \right) + \exp \left( \frac{ux}{D} \right) \text{erfc} \left( \frac{x+ut}{2\sqrt{D t}} \right) \right\}
\]

\[
- \exp(-\gamma t) \left\{ \exp \left[ \frac{x(u - \phi)}{2D} \right] \text{erfc} \left( \frac{x - \phi t}{2\sqrt{Dt}} \right) + \exp \left[ \frac{x(u + \phi)}{2D} \right] \text{erfc} \left( \frac{x + \phi t}{2\sqrt{D t}} \right) \right\}
\]
where,
\[
\phi = \left( u^2 - 4\gamma D \right)^{\frac{1}{2}}
\]
\[
\gamma = \text{Decay coefficient (day}^{-1})
\]

6 Development of numerical model

6.1 Calculation of advection

Considering the pure advection, the concentration, \( c(x, t) \) at any point and time is given by solution to relationship,

\[
\frac{\partial c(x, t)}{\partial t} + u(x, t) \frac{\partial c(x, t)}{\partial x} = 0
\]  

(6)

Where,
\[
x = \text{positive direction of flow;}
\]
\[
t = \text{time;}
\]
\[
u(x, t) = \text{time dependent flow velocity, (positive x direction).}
\]

Assuming that \( u(x, t) = u \), as constant, the formal solution to Eq.6 can be written as,

\[
c(x, t + \Delta t) = c(x - u\Delta t, t)
\]  

(7)

In which,
\[
\Delta t = \text{any interval of time.}
\]

‘i’ be an index of the computational points \( x_i \), \( i = 1, 2 \ldots \)

Denoting ‘n’ as the time level, such that, \( \Delta t = t_{n+1} - t_n \)

And denoting \( (x_i, t_n) \), by \( c^n_i \)

Knowing \( c^n_i \) for all ‘i’, the concentration at point \( c(x_i - u\Delta t, t_n) \) can be estimated, assuming linear variation of \( c(x, t) \) between \( x_{i-1} \) and \( x_i \). Thus,

\[
c(x_i - u\Delta t, t_n) = c^n_i - \left( \frac{u\Delta t}{x_i - x_{i-1}} \right) \left( c^n_i - c^n_{i-1} \right)
\]  

(8)

Then from Eq.6, direct solution gives

\[
c^n_{i+1} = c^n_i - \left( \frac{u\Delta t}{x_i - x_{i-1}} \right) \left( c^n_i - c^n_{i-1} \right)
\]  

(9)
The above method introduces several numerical damping when ratio is small. To reduce numerical damping usual procedure is to form a cubic polynomial in terms of concentrations at points, i-2, i-1, i, and i+1 and interpolating $c_i^{n+1}$ from this polynomial.

In the present “Two-point fourth order method” instead of considering four points only two points i, i-1 points are considered. A cubic polynomial is formed considering concentration at points i, i-1 as well as derivatives of concentrations at points, i and i-1. From this cubic polynomial, concentration at new time can be estimated using above procedure.

Denoting the derivatives of concentration at points i-1 and i by, $c_x(i-1, n)$ and $c_x(i, n)$ respectively, at time step n. Then the polynomial is formed as,

$$c(i,n-1) = a1.c(i-1,n) + a2.c(i,n) + a3.cx(i-1,n) + a4.cx(i,n)$$

Where,

$$a1=Cr^2(3-2Cr)$$
$$a2=1-a1$$
$$a3 = Cr^2 (1-Cr) (x_i-x_{i-1})$$
$$a4 = -Cr (1-Cr)^2 (x_i-x_{i-1})$$

$$Cr = \text{Courant number} = \frac{U\Delta t}{\Delta x}$$

To continue the calculations for the $n+2$th step it is necessary to calculate the derivatives of concentrations at the $n+1$th time step. These are calculated using similar procedure. The following polynomial is used to obtain the $cx$ values at the $n+1$th step.

$$cx(i,n+1) = b1.c(i-1,n) + b2.c(i,n) + b3.cx(i-1,n) + b4.cx(i,n)$$

Where,

$$b1 = 6Cr (Cr -1) / (x_i-x_{i-1})$$
$$b2=-b1$$
$$b3=Cr(3Cr-2)$$
$$b4 = (Cr-1)(3Cr-1)$$

This scheme introduces very little numerical diffusion and dispersion. In above calculations only advection is calculated. For the proper results it is necessary to calculate the diffusion and add the two results to get final value of concentration at a point. The method for calculating diffusion is described in next section.

6.2 Calculation of diffusion

In the solution of one-dimensional transport equation for ground water, the calculation of advection is immediately followed by the solution of equation,
\[
\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left( D_l \frac{\partial c}{\partial x} \right) \tag{10}
\]

Where, 
\(c, x, D_l\) are as defined earlier.

To calculate diffusion the finite-difference method used here is an explicit scheme as described by (Priessmann [3]). As per their method, Finite-Difference formulation of Eq.9 can be written as follows,

\[
c(i,n+1) - c(i,n) = \left( \frac{D_l \Delta t}{x_{i-1} - x_i} \right) \left[ \frac{c(i+1,n) - 2c(i,n) + c(i-1,n)}{(x_i - x_{i-1})} \right] \tag{11}
\]

The simulation proceeds by calculating an alternation series of advection and diffusion steps. The above method has been used to determine the concentration distribution in longitudinal direction for a field problem.

7 Applications

In this application the transport of a non-conservative constituent in a saturated porous media flow field is studied. The velocity of flow is 1.219 m/s. A dispersion coefficient of 7.616 m²/day, a grid spacing of 20 m is used. The time step of 2 days is used. For Case I the initial concentration is \(c(0,t) = 1\) units.

Graphs have been plotted for concentration versus distance and the concentration obtained by numerical scheme and analytical equations have been compared as shown in Fig.1. There is a good agreement between numerical and analytical solution for all time steps.

For case II an initial concentration is \(c(0,t) = c_0 e^\lambda\) in which \(c_0\) is 1 units and \(\lambda\) is \(-0.01\) day\(^{-1}\). Graphs have been plotted for concentration versus distance and the concentration obtained by numerical scheme and analytical equations have been compared as shown in Fig.2. There is a good agreement between numerical and analytical solution initially. Later Numerical scheme over predicts the concentration obtained by the analytical solution.
Figure 1: One-dimensional dispersion: comparison of numerical and analytical result.

Figure 2: One-dimensional dispersion: comparison of numerical and analytical result.
For Case III the initial concentration is \( c(0,t) = c_0 (1-e^{-\lambda t}) \) in which \( c_0 \) is 1 units and \( \lambda \) is 0.01 day\(^{-1}\). Graphs have been plotted for concentration versus distance and the concentration obtained by numerical scheme and analytical equations have been compared as shown in Fig.3. There is a good agreement between numerical and analytical solution initially. Later Numerical scheme over predicts the concentration obtained the analytical solution.

![Graph showing concentration versus distance for Case III](image)

Figure 3: One-dimensional dispersion: comparison of numerical and analytical result.

References


