A Semianalytical Solution of One-Dimensional Adveotive-Dispersive Solute Transport Under an Arbitrary Concentration Boundary Condition

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Abstract

By employing the principle of superposition, we offer a semianalytical solution for a one-dimensional advective-dispersive solute transport equation under an arbitrary concentration boundary condition. The technique is applicable to many other existing analytical solutions of solute transport problems.

Previous Work

The equation governing one-dimensional advective-dispersive transport in porous media, considering solute decay and adsorption, can be written as (Javandel et al., 1984, p. 14):

\[
D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \lambda RC = R \frac{\partial C}{\partial t}
\]

(1)

where $C$ is the solute concentration, $D$ is the dispersion coefficient, $v$ is the seepage velocity, $\lambda$ is the decay constant, $x$ and $t$ are the spatial and temporal coordinates, and $R$ is the retardation factor. For a linear sorption isotherm, $R = 1 + \rho K_d/n$, where $\rho$ is the bulk density of the porous medium, $K_d$ is the distribution coefficient, and $n$ is the porosity.

For a steady-state uniform flow in a homogeneous and isotropic porous medium, the velocity $v$ and the dispersion coefficient $D$ are constants, and the analytical solutions of equation (1) have been found under certain sets of initial and boundary conditions. Using the Laplace transform technique, Van Genuchten (1982) provided an analytical solution for a physical system with zero initial concentration in a semi-infinite domain; i.e.:

\[
C(x, t) = 0 \quad t = 0 \quad (2a)
\]

The boundary conditions are such that at the infinity from the source, there is no solute mass exchange with the system; i.e., mass flux is zero:

\[
\frac{\partial C(x, t)}{\partial x} = 0 \quad x = \infty \quad (2b)
\]

At the source location ($x = 0$), the solute flux equals the total solute entering the porous medium by dispersion and advection, with the strength of the source decaying exponentially with time as expressed by the following equation:

\[
\left[ -D \frac{\partial C}{\partial x} + vC \right]_{x=0} = vf(t) = v[H(t) - H(t - t_0)] C_0 \exp(-\alpha t) \quad (2c)
\]

where $H(\cdot)$ is the heaviside function, $t_0$ is the duration of the source, $C_0$ is the initial source strength, and $\alpha$ is the source decay constant. The solution of equations (1)-(2) is:

\[
C(x, t) = H(t) A(x, t) - H(t - t_0) A(x, t - t_0) \exp(-\alpha t_0) \quad \ldots (3a)
\]
where
\[ A(x, t) = C_0 \exp(-\alpha t) \left[ A_1(x, t) \left( l - \delta_{\alpha} \right) + A_2(x, t) \delta_{\alpha} \right] \]

... (3b)

where \( \delta_{\alpha} \) is the Kronecker delta function, and
\[ A_1(x, t) = \frac{v}{v + u} \exp \left( \frac{x(v - u)}{2D} \right) \text{erfc} \left( \frac{Rx - ut}{2(D\alpha)^{1/2}} \right) + \frac{v}{v - u} \exp \left( \frac{x(v + u)}{2D} \right) \text{erfc} \left( \frac{Rx + ut}{2(D\alpha)^{1/2}} \right) + \frac{v^2}{2DR(\lambda - \alpha)} \exp \left( \frac{vx}{D} + (\alpha - \lambda) t \right) \text{erfc} \left( \frac{Rx + vt}{2(D\alpha)^{1/2}} \right) \]

... (3c)

\[ A_2(x, t) = \frac{1}{2} \text{erfc} \left( \frac{Rx - vt}{2(D\alpha)^{1/2}} \right) + \left( \frac{v^2t}{\pi DR} \right)^{1/2} \exp \left( \frac{(Rx - vt)^2}{4D\alpha t} \right) - \frac{1}{2} \left( 1 + \frac{vx}{D} + \frac{v^2t}{DR} \right) \exp \left( \frac{vx}{D} \right) \text{erfc} \left( \frac{Rx + vt}{2(D\alpha)^{1/2}} \right) \]

... (3d)

\[ u = \left[ v^2 + 4DR(\lambda - \alpha) \right]^{1/2} \]

... (3e)

In some cases, such as where there is a fixed amount of radioactive decay material, the assumption of boundary condition (2c) may be reasonable. However, in general, the source of the solute is much more complicated; it often varies with time irregularly. A good example for such a source is the distribution of the atmospheric tritium concentration in the past 40 years, which has been shown to be the result of the nuclear bomb tests in the upper atmosphere. The tritium concentration changes drastically with both the global location and time. Figure 1 shows the tritium inflow with rainfall to the subsurface as a function of time at a specific location (Michel, 1989). In the case of the irregular solute inflow function such as the one illustrated in Figure 1, the analytical solution (3) cannot be directly applied, and one usually has to employ numerical methods such as the finite-difference, the finite-element, or the (modified) method of characteristics. Nevertheless, these numerical methods often experience some notorious numerical problems. We offer an alternative approach to the numerical methods. In practice, it is also efficient to utilize available and easily computed analytical solutions to perform an initial estimation of a solute transport problem, which sometimes can provide invaluable guidance for design of more complicated numerical modeling.

**Semianalytical Solution**

By using the mathematical property of the linearity of the governing equation, we apply the superposition principle to the existing solution (3) to obtain the exact solution for an arbitrary source function \( f(t) \) [see equation (2c)].

The technique is to decompose the source into a finite number of stepwise functions in the time domain as illustrated in Figure 1. Mathematically, it states
\[ f(t) = \sum_{i=1}^{n} f_i(t) [H(t - t_i) - H(t - t_{i+1})] \quad t_i < t \leq t_{i+1} \]

... (4)

where \( f_i \) is the source concentration during the time interval \( \Delta t_i \) (= \( t_{i+1} - t_i \)), and \( n \) is the number of the time interval chosen.

Each stepwise source function is equation (2c) alike, with \( \alpha \), the source decay constant, set to zero. This function, with the initial and boundary conditions (2a) and (2b) and the governing equation (1), can lead to the analytical solution in the same form as equation (3). For instance, the concentration distribution \( C(x, t - t_i) \), responding to a stepwise source boundary \( f(t_i) \) (Figure 1) during the time interval \( \Delta t_i \) (= \( t_{i+1} - t_i \)), can be fully described by equations (3a)-(3e) with a starting time shifted from 0 to \( t_i \).

The total concentration distribution \( C_i(x, t) \), for a general source strength of \( f(t) \) described by equation (4), can be integrated as:
\[ C_i(x, t) = \sum_{i=1}^{n} H(t - t_i) C_i(x, t - t_i) \]

... (5)

where \( C_i \) is the analytical solution (3) for a stepwise concentration boundary condition.

The analytical solution (3) has been programmed into a code ODAST (Javandel et al., 1984, Appendix B). We made a few modifications on ODAST to implement equations (4) and (5) for irregular concentration boundary conditions. Specifically, we inserted several lines of code to compute equation (4) so that the main program will call this new block if an irregular boundary condition in the form of equation (4) is desired. To verify the modified ODAST program, we conducted a set of numerical experiments. Javandel et al. (1984) tabulated a series of numerical results in Appendix A of their book. We compared the results of concentration versus time and concentration versus distance from the modified program with the values in the tables (Javandel et al., 1984) for different \( v \), \( D \), \( \lambda \), \( R \), \( \alpha \), \( C_0 \), and \( t_0 \). Identical results are obtained. For those who are interested in obtaining the modified program, please send to either author a floppy and a stamped, self-addressed envelope.

![Fig. 1. An illustration of the source boundary condition as an irregular function of time and the superposition of the stepwise functions.](image-url)
Discussion

As an example, we use the irregular boundary condition, plotted in Figure 1, to analyze tritium transport in a hypothetical unsaturated porous medium. The unsaturated zone is conceptualized as 500 meters thick of homogeneous isotropic rock with a steady-state downward uniform infiltration velocity \( v \) of 10 m/yr. We further assume that the longitudinal dispersion coefficient \( D \) is \( 10^{-7} \) m\(^2\)/s and that there is no retardation during the tritium transport. The radioactive decay constant \( \lambda \) for tritium is 0.0556 yr\(^{-1}\). The resulting tritium concentration distributions in rock in different years are illustrated in Figure 2. It is interesting to note that the peak concentration of 1700 TU in the source input in the year 1963 resulted in a peak concentration of 238 TU at 255 meters below the surface as time advances to the year 1988.

The downward migration and decay nature of the tritium fluxes can be quantitatively illustrated by this simple technique.

The proposed technique allows the application of the existing analytical solution to more complicated and realistic physical problems, such as the transport of the environmental isotopes in porous media. It provides an efficient and accurate tool. In fact, as the number of time segments increases, the solution will approach the exact solution. From the computational technique point of view, it possesses some advantages over the numerical methods. One advantage is that it avoids the notorious potential numerical problems such as numerical dispersion, oscillation, instability, and inaccuracy. A second advantage is that it is not confined to the limited application of most analytical solutions whose boundary conditions are usually highly simplified. The proposed superposition technique can easily be applied to any other existing analytical solution, including some for solute transport in more complicated two- and three-dimensional flow systems. Although the current illustration is limited to the one-dimensional uniform flow problem, it considers general solute transport mechanisms of advection, dispersion, radioactive decay, and chemical adsorption. It is also very easy to use.

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References