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Solute transport with longitudinal and transverse diffusion in temporally and spatially dependent flow from a pulse type source

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ABSTRACT

Molecular transverse diffusion through unsteady and heterogeneous medium is accounted for in solute mass transport originating from a uniform pulse-type stationary point-source. The corresponding two-dimensional advection–dispersion equation with variable coefficients is solved by the explicit finite difference method. The heterogeneity of the medium is described by a position dependent linear non-homogeneous expression for velocity with unsteady exponential variation with time. Variation of the dispersion parameter due to heterogeneity is considered proportional to square of the velocity. Results are compared to analytical solutions reported in the literature and good agreement is found. The explicit finite difference method is shown to be effective and accurate for solving the related two-dimensional advection–dispersion equation with variable coefficients in semi-infinite media, which is especially important when arbitrary initial and boundary conditions are required.

1. Introduction

The degradation of air, water and soil has renewed research interest in the field of solute transport by flow media. This transport can be described by the advection–dispersion equation. It is a partial differential equation in space and time that is of much significance in such diverse disciplines as chemical and petroleum engineering or bio and soil physics [1]. For example, the advection–dispersion equation can be used to determine the pollutant concentration downstream from intended mining operations in order to predict and plan how to reduce their environmental footprint.

Lindstrom and Boersma [2] have reviewed analytical solutions for one-dimensional solute transport through media idealized as homogeneous. However, the actual solute permeation through air, soil or groundwater tends to be position dependent. To account for this heterogeneity, spatially-dependent dispersion and velocity have to be considered. This has been solved analytically for special cases in one dimension [3–8]. Numerical solutions are required for cases that are more general and for problems in two or three dimensions [9–16]. Dehghan [12] employed weighed explicit finite difference method (EFDM) for one-dimensional advection–dispersion equation with increased accuracy of the obtained numerical results if compared to that of standard finite difference methods. Karahan [13] used implicit finite difference method (IFDM) for one-dimensional advection–dispersion equation using spreadsheets. Walter et al. [17] used Crank–Nicholson central difference scheme in one dimension to model soil solute release into runoff with infiltration. In the 1970s and 1980s, IFDMs were generally preferred over EFDMs. This trend has been changing with the advancement of computers, shifting the emphasis to EFDMs. Being often unconditionally stable, the IFDM allows larger step lengths. Nevertheless, this does not translate into IFDM's higher computational efficiency because extremely large matrices must be manipulated at each calculation step. EFDM is also simpler in addition to being computationally more efficient. We have demonstrated in our recent work [18,19] the effectiveness of the EFDM in solving one-dimensional advection–dispersion equation with variable coefficients. This is now expanded to two dimensions in semi-infinite and horizontal media with a small-order heterogeneity. The heterogeneity is represented by interpolating velocity linearly as a non-homogeneous increasing function of position over the finite domain for evaluating concentration values. Dispersion unsteadiness is another variation that is allowed in order to accommodate the finding by Freeze and Cherry [20] that the dispersion is proportional to the nth power of velocity, with the exponent n ranging from 1 to 2.

Expressions for velocity and dispersion are written in this text in degenerate form [21,22] and the solution is presented to show solute transport along both the longitudinal and transverse directions. A significant solute transport is noted along transverse direction even at very low transverse velocity and dispersivity relative to their longitudinal counterparts. This shows that the two-dimensional model is more appropriate than a one-dimensional model.

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2. Advection–dispersion equation

Let solute particles of a pollutant be entering a body of air, soil or water (including groundwater) at uniform rate at some location, continuously for a fixed amount of time. In other words, there is a stationary point-source emitting a uniform pulse of pollutants (Fig. 1). This could be a smokestack, volcano, sewage outlet, or infiltration from a garbage dump, septic tank or tailings pond that is uniformly active for a fixed period of time and then ceases. From such point-source as the origin of mutually perpendicular horizontal x and y axes ($0 \leqslant x < \infty$; $0 \leqslant y < \infty$) defining a horizontal plane, solute particles are transported by diffusion and convection mainly downstream in the longitudinal direction chosen for the x-axis (with the y-axis along the transverse direction).

Let the velocity components of the flow field in x and y directions at position (x,y) in the horizontal plane be $u(x,t)$ and $v(y,t)$, respectively. Both satisfy the Darcy law if the medium is porous; or laminar flow conditions otherwise. Further, let $D_x(x,t)$ and $D_y(y,t)$ be longitudinal and transverse components of the solute dispersivity parameter at the same position, respectively [23]. The linear advection–dispersion partial differential equation in two-dimensional horizontal plane medium may be written in the following general form:

$$\frac{\partial C(x,y,t)}{\partial t} = \frac{\partial}{\partial x}\left(D_x(x,t)\frac{\partial C(x,y,t)}{\partial x} - u(x,t)C(x,y,t)\right) + \frac{\partial}{\partial y}\left(D_y(y,t)\frac{\partial C(x,y,t)}{\partial y} - v(y,t)C(x,y,t)\right) \quad (1)$$

where $C(x,y,t)$ is the dispersing solute concentration of the pollutant being transported along the flow field through the medium at a position (x,y) at time t.

To solve the two-dimensional advection–dispersion Eq. (1) analytically [24], a set of initial and boundary conditions are needed. Initially, the semi-infinite medium is considered solute free until introducing a uniform pulse from the pollution source at the origin of the x–y axes, lasting until (ceasing at) time t_0. Flux type homogeneous conditions are assumed at the far ends of the medium, along both directions. Thus, the initial condition and boundary conditions are [23]:

$$C(x,y,t) = 0, \quad x \geqslant 0;\ y \geqslant 0,\ t = 0 \quad (2)$$

$$C(x,y,t) = \begin{cases} C_0, & x = 0; y = 0; \quad 0 < t \leqslant t_0 \\ 0, & x = 0; y = 0; \quad t > t_0 \end{cases} \quad (3)$$

$$\frac{\partial C(x,y,t)}{\partial x} = 0,\ x \to \infty; \quad \frac{\partial C(x,y,t)}{\partial y} = 0,\ y \to \infty;\ t \geqslant 0 \quad (4)$$

where C_0 is the reference concentration representing the input concentration emitted uniformly by the source. Because the medium is assumed to be heterogeneous, the two perpendicular velocity components of the flow field are considered to be linear functions of respective coordinates (x,y) over the finite domain in which concentration values are evaluated. Each of the two linear functions can thus account for a small increase in velocity across the finite region. Further, velocity is also considered temporally dependent (in the same functional manner) in both, the longitudinal and transverse directions. Thus, expressions for velocity components are written in the degenerate form as:

$$u(x,t) = u_0 f_1(mt)(1+ax); \quad v(y,t) = v_0 f_1(mt)(1+by) \quad (5)$$

where a and b are the heterogeneity parameters along longitudinal and transverse directions, respectively. Their dimension is the inverse of length [24]. Different values for the pair (a,b) represent media of different heterogeneity. The other coefficient, m, represents the unsteadiness parameter. Its dimension is the inverse of time. Scheidegger [25] found that the solute dispersion parameter was proportional to square of the velocity when there was enough time in each flow channel for appreciable mixing to take place by molecular transverse diffusion. The consideration of transverse diffusion makes the dispersion problem two-dimensional. Hence, the variation in dispersion due to heterogeneity is proportional to square of the respective velocity. Hence:

$$D(x,t) = D_{x0} f_2(mt)(1+ax)^2, \quad D(y,t) = D_{y0} f_2(mt)(1+by)^2 \quad (6)$$

In the particular case of $f_2(m,t) = f_1^2(mt)$, Scheidegger's approach can be applied [25]. Namely expressions $(1 + ax)$, $(1 + by)$, $f_1(mt)$ and $f_2(mt)$ are non-dimensional; hence in Eq. (5), the coefficients u_0, v_0 may be referred to as uniform longitudinal and transverse velocity components, respectively (with dimension of speed). Similarly in Eq. (6), D_{x0} and D_{y0} may be referred to as the initial longitudinal and transverse dispersion coefficients, respectively, with dimension of $m^2\ s^{-1}$. It is ensured that $f(mt) = 1$ for $m = 0$ or $t = 0$ ($m = 0$ represents the steady flow and steady solute transport while $t = 0$ represents the initial state).

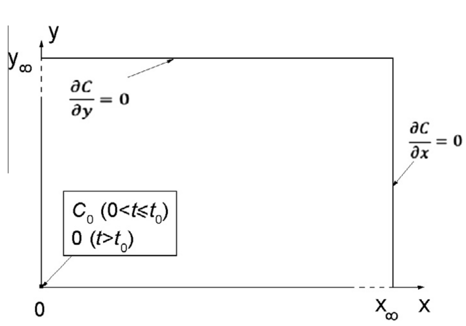

Fig. 1. Conceptual schematic of the physical model for solute transport from a pulse type source.

3. Analytical solution of advection–dispersion equation

Analytical solution of the advection–dispersion equation (1), subject to initial condition (2) and boundary conditions (3) and (4), is [23]:

$$C(x,y,t) = F(x,y,t); \quad 0 < t \leqslant t_0 \quad (7a)$$

$$C(x,y,t) = F(x,y,t) - F(x,y,t-t_0); t > t_0 \quad (7b)$$

where:

$$F(x,y,t) = \frac{C_0}{2}\left\{\exp\left[\left(-\frac{U}{U-D}\eta\right)\right] erfc\left[\frac{\eta}{2(1-\lambda)\sqrt{DT^*}} - \mu(1-\lambda)\sqrt{T^*}\right] + \exp\left[\left(-\frac{U^2}{D(U-D)}\eta\right)\right] erfc\left[\frac{\eta}{2(1-\lambda)\sqrt{DT^*}} + \mu(1-\lambda)\sqrt{T^*}\right]\right\} \quad (8)$$

and where:

$$\eta = Z\frac{f_1(mt)}{f_2(mt)}f_3(mt), \quad Z = \ln[(1+ax)(1+by)],$$

$$f_3(mt) = 1 - \lambda\frac{f_2(mt)}{f_1(mt)}, \quad \lambda = \frac{D}{U},$$

$$D = a^2 D_{x0} + b^2 D_{y0}, U = au_0 + bv_0,$$

$$\mu = \sqrt{\left(\gamma U + \frac{U^2}{4D}\right)} = \frac{U}{2\sqrt{D}}\frac{U+D}{U-D}, \quad T^* = \int_0^t f_1(mt)dt$$

Solution (7) may also be used for the following set of temporally dependent functions [23]: