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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 $\upsilon(y,t)$, 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:

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

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]:

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

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

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

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:

$$u(x,t) = u_0 f_1(mt)(1+ax); \quad \upsilon(y,t) = \upsilon_0 f_1(mt)(1+by) \tag{5}$$

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:

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

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, υ_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).

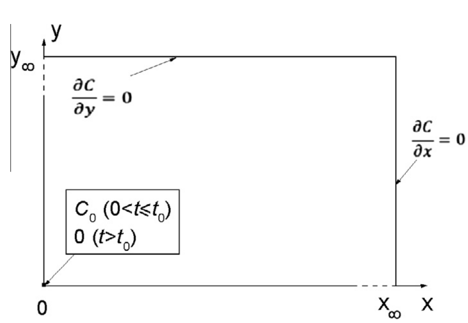

Fig. 1. Conceptual schematic of the physical model for solute transport from a pulse type source.

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]:

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

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

where:

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

and where:

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

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

$$D = a^2 D_{x0} + b^2 D_{y0}, U = au_0 + b\upsilon_0,$$

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

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

$$f_1(mt) = \exp(-mt); \quad f_2(mt) = \exp(mt) \tag{9}$$

In other words, the solution obtained for exponentially decelerating dispersion along exponentially accelerating velocity is also valid in case of the reverse-unsteady nature of the two parameters. Further, in each of the two situations, $f_1(mt)$ and $f_2(mt)$ are inverse of each other. It may be verified [23] that as far as the exponential nature of the unsteady variation is considered, the temporally dependent functions could be in the following form:

$$f_2(mt) = f_1^n(mt)) \tag{10}$$

for any value of the exponent n.

3.1. Steady solute transport along steady flow through inhomogeneous medium

This case may be obtained for $m = 0$, when $f_1(mt) = 1$, $f_2(mt) = 1$, $f_3(mt) = 1 - \lambda = (U-D)/U$, $\eta = [(U-D)/U]\ln[(1+ax)(1+by)]$ and $t = T^*$. Thus in this case, analytical solution of advection–dispersion equation (1) is given by Eqs. (7a,b), where the function $F(x,y,t)$ in Eq. (7) becomes:

$$F(x,y,t) = \frac{C_0}{2}\left\{[(1+ax)(1+by)]^{-1} erfc\left[\frac{\ln((1+ax)(1+by))}{2\sqrt{Dt}} - \frac{U+D}{2\sqrt{D}}\sqrt{t}\right] + [(1+ax)(1+by)]^{U/D} erfc\left[\frac{\ln((1+ax)(1+by))}{2\sqrt{Dt}} + \frac{U+D}{2\sqrt{D}}\sqrt{t}\right]\right\} \tag{11}$$

3.2. Case when the unsteadiness of dispersion is proportional to square of velocity through inhomogeneous medium

This case is achieved when $f_2(mt) = f_1^2(mt)$. It makes the solute dispersion along longitudinal or transverse direction proportional to square of the respective velocity component [25]. Then, $f_3(mt) = (1 - \lambda f_1(mt))$. Thus in the solution given by (7a,b), the function $F(x,y,t)$ will be the same as that given by Eq. (8), and then $\eta = Z[1 - \lambda f_1(mt)]/f_1(mt)$.

3.3. Case when the unsteadiness of dispersion is directly proportional to the velocity through inhomogeneous medium

This case is achieved when $f_2(mt) = f_1(mt)$. Then, $f_3(mt) = (1 - \lambda)$ and in the solution (7a,b) the function $F(x,y,t)$ is as given by Eq. (11) except that T^* replaces t.

4. Numerical method

Analytical solutions of advection–dispersion equations have been reported for specific initial and boundary conditions. This restriction, compounded with their complexity, limits their applicability. Numerical methods, on the other hand, are generally applicable with arbitrary initial distribution and boundary conditions [18,19,26,27]. In order to solve equation (1) by the explicit difference method, this equation is first rewritten in the following form:

$$\begin{aligned}\frac{\partial C(x,y,t)}{\partial t} = &\left(\frac{\partial D_x(x,t)}{\partial x}\frac{\partial C(x,y,t)}{\partial x} + D_x(x,t)\frac{\partial^2 C(x,y,t)}{\partial x^2}\right) \\ &- \left(\frac{\partial u(x,t)}{\partial x}C(x,y,t) + u(x,t)\frac{\partial C(x,y,t)}{\partial x}\right) \\ &+ \left(\frac{\partial D_y(y,t)}{\partial y}\frac{\partial C(x,y,t)}{\partial y} + D_y(y,t)\frac{\partial^2 C(x,y,t)}{\partial y^2}\right) \\ &- \left(\frac{\partial v(x,t)}{\partial y}C(x,y,t) + v(x,t)\frac{\partial C(x,y,t)}{\partial y}\right)\end{aligned} \tag{12}$$

Using equation (5) for $u(x,t)$ and $v(y,t)$ and equation (6) for $D_x(x,t)$ and $D_y(y,t)$, equation (12) can be written as:

$$\begin{aligned}\frac{\partial C(x,y,t)}{\partial t} = &\left(2aD_{x0}f_2(mt)(1+ax)\frac{\partial C(x,y,t)}{\partial x} + D_{x0}f_2(mt)(1+ax)^2\frac{\partial^2 C(x,y,t)}{\partial x^2}\right) \\ &- \left(au_0 f_1(mt)C(x,y,t) + u_0 f_1(mt)(1+ax)\frac{\partial C(x,y,t)}{\partial x}\right) \\ &+ \left(2bD_{y0}f_2(mt)(1+by)\frac{\partial C(x,y,t)}{\partial y} + D_{y0}f_2(mt)(1+by)^2\frac{\partial^2 C(x,y,t)}{\partial y^2}\right) \\ &- \left(bv_0 f_1(mt)C(x,y,t) + v_0 f_1(mt)(1+by)\frac{\partial C(x,y,t)}{\partial y}\right)\end{aligned} \tag{13}$$

In order to solve equation (13) by the explicit finite difference method, the central difference scheme is used to represent the terms $(\partial^2 C(x,t)/\partial x^2)$, $(\partial^2 C(y,t)/\partial y^2)$, $(\partial C(x,t)/\partial x)$ and $(\partial C(y,t)/\partial y)$ and a forward difference scheme for the derivative term $(\partial C(x,t)/\partial t)$ [28]. With these substitutions, equation (13) transforms into:

$$\begin{aligned}C_{i,j,k+1} = &(L_{i,k} + M_{i,k})C_{i+1,j,k} + (M_{i,k} - L_{i,k})C_{i-1,j,k} + (N_{j,k} + P_{j,k})C_{i,j+1,k} \\ &+ (P_{j,k} - N_{j,k})C_{i,j-1,k} + (1 - 2M_{i,k} - 2P_{j,k} - K_k)C_{i,j,k}\end{aligned} \tag{14}$$

where indexes i, j and k refer to the discrete step lengths Δx, Δy and Δt for the coordinate x, coordinately y and time t, respectively, and where:

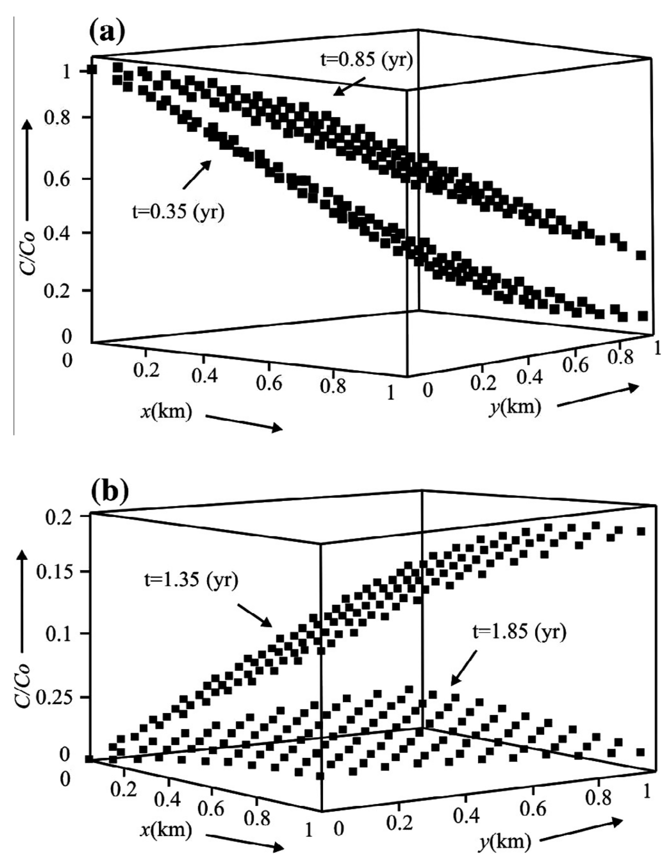

Fig. 2. Numerical solution (solid squares) of the solute transport due to decelerating dispersion along accelerating flow through a medium of linearly increasing heterogeneity for (a) source active ($0 < t \leqslant t_0$), and (b) source inactive ($t > t_0$; deactivates at t_0 = 1.0 year). Open squares represent the analytical solution; they overlap with solid squares because deviations are small.

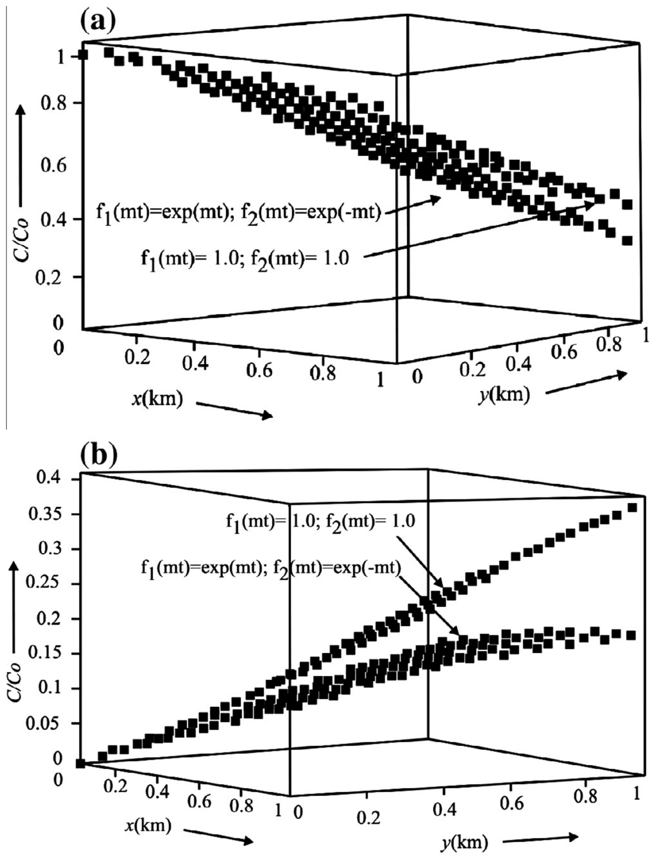

Fig. 3. Numerical solution (solid squares) of the solute transport due to (i) decelerating dispersion along accelerating flow, and (ii) steady dispersion along steady flow, both through the same medium, (a) at $t = 0.85$ years when the source is active, and (b) at $t = 1.85$ years when the source is inactive (deactivates at $t_0 = 1.0$ year). Open squares represent the analytical solution; they overlap with solid squares because deviations are small.

$$L_{i,k} = \frac{E_k(1+ax_i)\Delta t}{2\Delta x}, \quad M_{i,k} = \frac{G_k(1+ax_i)^2\Delta t}{\Delta x^2}$$
$$N_{j,k} = \frac{F_k(1+by_j)\Delta t}{2\Delta y}, \quad P_{j,k} = \frac{H_k(1+by_j)^2\Delta t}{\Delta y^2}$$
$$E_k = B_1 f_2(mt_k) - u_0 f_1(mt_k)$$
$$F_k = B_3 f_2(mt_k) - \upsilon_0 f_1(mt_k)$$
$$G_k = D_{x0} f_2(mt_k)$$
$$H_k = D_{y0} f_2(mt_k)$$
$$B_1 = 2aD_{x0}, \quad B_2 = au_0, \quad B_3 = 2bD_{y0}, \quad B_4 = b\upsilon_0$$

The truncation error for the difference equation (14) is $O(\Delta t, \Delta x^2, \Delta y^2)$. Using a small-enough value of Δt, Δx and Δy, the truncation error can be reduced until the accuracy achieved is within the error tolerance [28].

The initial condition (2) for Eq. (14) can be expressed in the finite difference form as:

$$C_{i,j,0} = 0, \quad x \geq 0; \; y \geq 0 \quad t = 0 \tag{15}$$

Boundary conditions (3) and (4), rewritten in the finite difference form, are:

$$C_{0,0,k} = \begin{cases} C_0, & x = 0; \; y = 0; \quad 0 < t \leqslant t_0 \\ 0, & x = 0; \; y = 0; \quad t > t_0 \end{cases} \tag{16}$$

$$C_{N,j,k} = C_{N-1,j,k}, x \to x_\infty; \quad C_{i,R,k} = C_{i,R-1,k}, \; y \to y_\infty; \quad t \geq 0 \tag{17}$$

where $N = x_\infty/\Delta x$ and $R = y_\infty/\Delta y$ are the grid dimension in the x and y directions, respectively, x_∞ is the distance in direction x at which $\partial C/\partial x = 0$ and y_∞ is the distance in direction y at which $\partial C/\partial y = 0$ (x_∞ and y_∞ replaces $x \to \infty$ in equation (4)). In this manner, solute concentration can be determined at different times. A typical solution run takes up to 3 s on the Intel (R) Core (TM) i3 CPU 540 @ 3.07 GHz personal computer for the longest time analyzed (1.85 year).

5. Numerical and analytical results

Numerical solution of Eq. (12) using EFDM is obtained for the same set of input data previously used by Yadav et al. [23]. The concentration values $C(x,y,t)$ are determined assuming reference concentration $C_0 = 1.0$, in a finite domain along longitudinal and transverse directions $0 \leqslant x \leqslant 1$ km and $0 \leqslant y \leqslant 1$ km, respectively. In Eq. (17), we used $x_\infty = y_\infty = 20$ km as the distances at which there is no further change in the concentration $C(x,y,t)$ (the same value for x_∞ and y_∞ is used for all problems analyzed). Increasing x_∞ and y_∞ further affected the solution only slightly but greatly increased the grid size and, therefore, the computation time. In the numerical calculations, the step lengths $x = y = 0.1$ km and $t = 0.00005$ (year) have been used to achieve the stability of the finite difference scheme. By setting $a = b = 0.1$ km^{-1}, the medium is assigned the same heterogeneity in both directions. The values for initial velocity and dispersion coefficient components are taken as $u_0 = 1.05$ km/year, $\upsilon_0 = 0.15$ km/year, $D_{x0} = 1.1$ km^2/year and $D_{y0} = 0.1$ km^2/year. The unsteadiness parameter is chosen as $m = 0.1$ year^{-1}. The source of pollution is deemed to have been eliminated (deactivated) at time $t_0 = 1.0$ year. It is also used that $f_1(mt) = \exp(mt)$ and $f_2(mt) = \exp(-mt)$, implying that the velocity

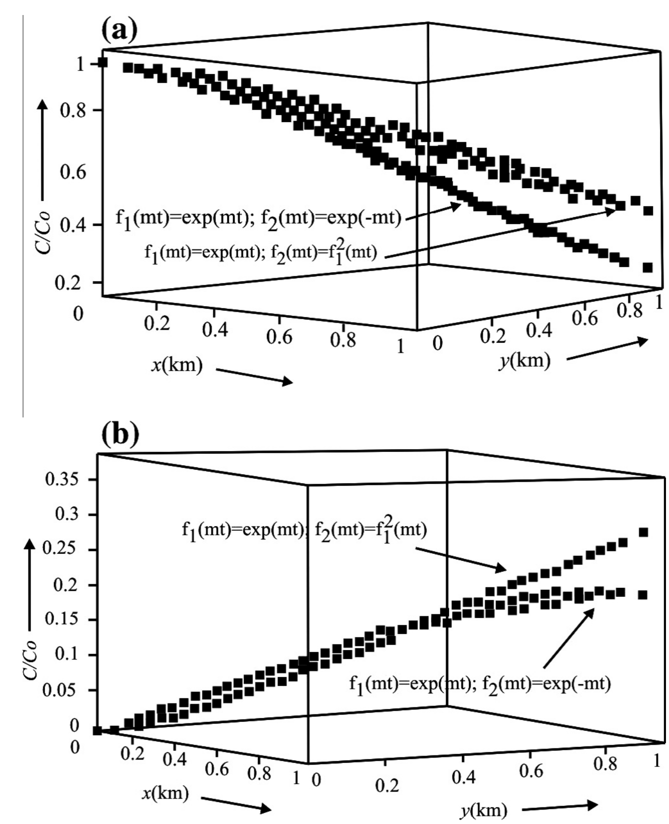

Fig. 4. Numerical solution (solid squares) of the solute transport due to (i) decelerating dispersion along accelerating flow, and (ii) dispersion being square of the accelerating velocity, both through the same medium, (a) at $t = 0.85$ years when the source is active, and (b) at $t = 1.85$ years when the source is inactive (deactivates at $t_0 = 1.0$ year). Open squares represent the analytical solution; they overlap with solid squares because deviations are small.

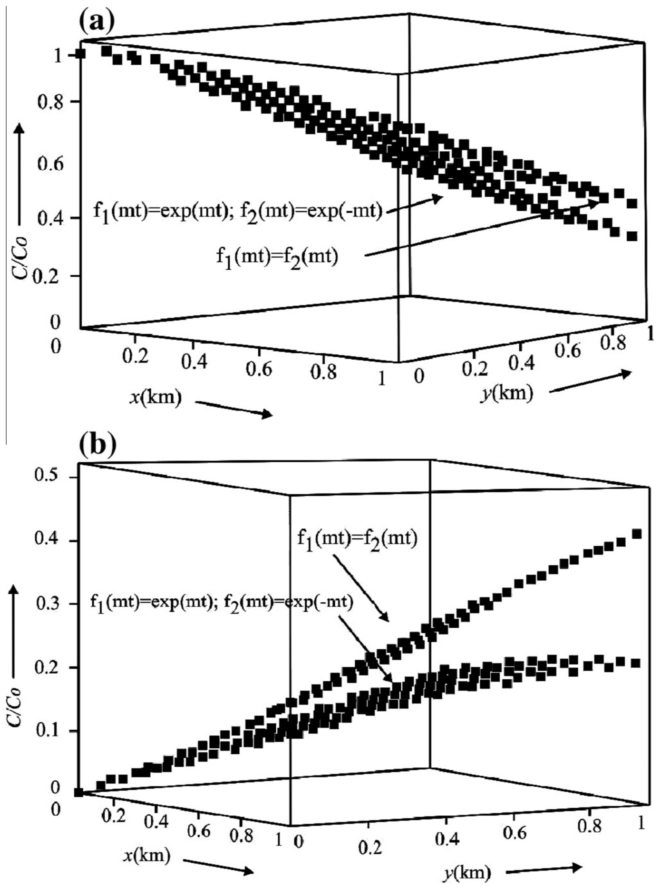

Fig. 5. Numerical solution (solid squares) of the solute transport due to (i) decelerating dispersion along accelerating flow, and (ii) accelerating velocity and dispersion, both through the same medium, (a) at $t = 0.85$ years when the source is active, and (b) at $t = 1.85$ years when the source is inactive (deactivates at $t_0 = 1.0$ year). Open squares represent the analytical solution; they overlap with solid squares because deviations are small.

of the flow accelerates exponentially whereas the solute dispersivity decelerates exponentially. In Fig. 2, filled squares represent numerical solution (14) of the advection–dispersion equation (1) while open squares represent analytical solution (7) of the advection–dispersion equation (1). A good agreement between the numerical and analytical solution is obtained. Due to the insignificance of deviations that are within 0.04% (the same accuracy has been achieved in all problems analyzed), solid squares overlapped open squares, thus the latter cannot be distinguished in the figures. Fig. 2a shows solute transport from the point source along the longitudinal and transverse directions in the presence of the source of pollution ($t < t_0$), at times $t = 0.35$, and $t = 0.85$ years. The input concentration $C(x = 0, y = 0, t) = C_0 = 1.0$ is assumed at both times. It attenuates with position and time. Similarly, Fig. 2b illustrates the solute transport from the point source along the two directions once the source of the pollution has been eliminated ($t > t_0$), at $t = 1.35$ and 1.85 years. The input concentration remains zero. This figure shows the trend of the polluted domain becoming concentration-free with position and time. From Fig. 2a and b, it can be observed that the recovery process is faster.

The solute transport with the source active and the subsequent recovery (with the source inactive), in the case of the exponentially decelerating dispersivity governed by $f_2(mt) = \exp(-mt)$ along exponentially accelerating flow described by $f_1(mt) = \exp(mt)$, are compared for the following three cases (discussed earlier in this text):

(i) $f_2(mt) = f_1(mt) = 1$, i.e. uniform dispersion along uniform flow,
(ii) $f_1(mt) = \exp(mt)$, $f_2(mt) = f_1^2(mt)$, i.e. the solute dispersion is proportional to square of the velocity, and
(iii) $f_1(mt) = \exp(mt)$, $f_2(mt) = f_1(mt)$, i.e. exponentially accelerating dispersion along exponentially accelerating velocity.

These comparisons are shown in Figs. 3–5. The figures suffixed (a) are for $t = 0.85$ year ($<t_0$) and those suffixed (b) are for $t = 1.85$ year ($>t_0$). It can be observed from Figs. 3–5 that the rise of the solute concentration while the source is active is faster than the recovery process (source inactive) in all three cases. Ranked by this speed rising, the three cases would be ordered as i–ii–iii when the source is active, and iii–ii–i when the source is inactive.

One can conclude that neither the transverse component of velocity nor that of dispersivity could be neglected for realistic assessment of solute transport. A two-dimensional model is more accurate than a one-dimensional model that does not account for the transverse diffusion. It could be misunderstood that as the expression $f(mt) = \exp(mt)$ tends to infinity with $t \to \infty$, dispersion and velocity would both increase enormously. As can be observed in the figures, however, the concentration gradient with position tends to zero as time increases; hence, the solute transport ceases within a finite period of time. Moreover, the unsteadiness parameter m is small, much less than unity.

6. Conclusion

Using the explicit finite difference method, solutions are obtained for dispersion through a heterogeneous horizontal semi-infinite medium. The heterogeneous nature of the medium is described by a position dependent linear non-homogeneous expression for velocity with unsteady exponential variation with time. Neither velocity nor dispersion are zero at the origin. Numerical results are compared to analytical solutions reported in the literature and good agreement is found. The transverse component of velocity and that of dispersivity are both significant enough to justify the application of the two-dimensional model.

The explicit finite difference method is found to be effective and accurate for solving the two-dimensional advection–dispersion equation with variable coefficients in semi-infinite (heterogeneous) media. It can be used with arbitrary initial and boundary conditions, as well as with different variations of dispersion and velocity, for which analytical solutions are not available.

Acknowledgments

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