Numerical Solution of the Two-Dimensional Time-Dependent Transport Equation

Khaled Ismail Hamza[1]

[1] The Hashemite University, Zarqa – Jordan

EXTENDED ABSTRACT

A two-dimensional model, which provides approximate description of time-dependent transport, is presented. The model involves solution of the advection-dispersion equation but with the dispersion coefficient dependent on the travel time of the solute from a single source. The governing equation, which includes, a time varying dispersion coefficient, linear equilibrium adsorption, and first order reaction, is modeled. In this study, particular solution from various dispersion functions and mass injection scenarios is presented. Theses include linear, asymptotic, and exponential variation of the dispersion functions and continuous mass injection. Three scenarios were considered to investigate solute migration with time-dependent dispersion coefficient. In all scenarios, all geometric, physical and transport parameters were maintained constant but dispersion coefficient was changed. The results could model transport of solute in a hydrologic system characterized by a dispersion coefficient that varies as a function of travel time from the input source. Based on numerical simulations, equiconcentration lines were drawn to characterize solute distribution. The developed solution should be applicable to a broad variety of solute transport problems, especially those in heterogeneous porous media.

INTRODUCTION

Non-reactive solute transport in saturated porous media is described by classical convection-dispersion model in which the transport coefficients (dispersion coefficients and velocity) are uniform constants. However, there has been an increased awareness in recent years about the inadequacy of the advection-dispersion equation in describing solute transport in hydrologic systems. It, however, fails to describe solute transport in saturated porous media if significant spatial availability in the fluid velocity field exists (Sposito et al., 1986). Field evidence and experimental studies have suggested that the dispersion coefficient is not constant but apparently increasing as a function of travel time or equivalently (Sauty, 1980; Pickens and Grisak, 1981a).

Gelhar et al., (1979) reported that the dispersion depends on the travel time and that it increases until it reaches an asymptotic value. Theoretical deterministic analysis by Güven et al. (1984) has also established that the dispersivity in a stratified aquifer is dependent on time. Sposito and Barry (1987) have shown that the time-dependent dispersion coefficients are a general property of the stochastic velocity process, the initial conditions, and the porous medium. Therefore a time-dependent dispersion model can be used to provide an approximate description of scale-dependent transport. Analytical solutions to the transport equation with time-dependent coefficients (Barry and Sposito, 1989), distance-dependent with linear variation (Yates, 1990; Serrano, 1992), and asymptotic variation (Hamza, 2000) were presented.

Barry and Sposito (1989) had published an analytical solution for the convection-dispersion with time-dependent coefficients in a semi-infinite domain. Their solution is based on the results of Cannon (1984) and involves an implicit equation, a Volterra integral equation of the second kind, which must be solved numerically. Basha and El-Habel (1993) developed an analytical model based on the advection-dispersion equation with the dispersion coefficient dependent on the travel time of the solute from a single input source. They assumed an infinite domain. The model was developed for linear, exponential and asymptotic variation of the dispersion functions and instantaneous as well as continuous mass injection.

In this study, the approach of Pickens and Grisak (1981b) is followed where the scale effect is handled by time-dependent dispersion coefficient of arbitrary form. The dispersion coefficient in the numerical model is mathematically assumed to be dependent on the travel time of the solute transport rather than dependent on the mean travel distance as assumed by Yates (1992) and by Pickens and Grisak (1981b). Since the mean travel distance is directly proportional to mean travel time in a constant velocity field, the two formulations are equivalent (Basha and El-Habel, 1993). The model is developed for constant, linear, exponential, and asymptotic variation and only the latter is studied since it is of more practical importance.

BASIC EQUATIONS

The governing differential equations describing flow and transport of solute injected in an infinite medium with time-dependent dispersion, linear equilibrium adsorption and first-order decay are:

Flow equation

$$\frac{\partial(\theta\rho)}{\partial t} = \nabla.\rho\left[K_{ij}\left(\nabla\psi + \rho_r \nabla z\right)\right] + P\rho_{in} \tag{1}$$

Transport equation:

$$\frac{\partial}{\partial t}(\theta C) = \nabla.\left[CK_{ij}\left(\nabla\psi + \rho_r\nabla z\right)\right] + \nabla.\left(\theta D^*(t).\nabla C\right) - K_d\,\rho_b\frac{\partial C}{\partial t} - \theta\lambda C + PC_{in} \tag{2}$$

where θ is the porosity of the aquifer medium; ρ is the density of mixed fluid, which is defined as $\rho = \rho_o + \beta\left(C - C_o\right)$; ρ_o is freshwater density, C is solute concentration, C_o is freshwater concentration and β is a constant, K_{ij} is the hydraulic conductivity tensor (i,j=1,2), ρ_r is the relative density and is defined as $\rho_r = \rho/\rho_o - 1$, ψ is the equivalent freshwater head, defined as $\psi = p/(\rho_o g) + z$, p is the pressure, z is elevation and g is the gravitational acceleration, P is the injection rate through a vertical well, and ρ_{in} is the density of the injected water. $D^*(t)$ is the time-dependent dispersion coefficient, K_d is the distribution coefficient ρ_b is the bulk density of porous medium, λ is the first-order decay coefficient, and C_{in} is the solute concentration of the injected water.

For the sake of contrast, the actual head is $\phi = p/(\rho g) + z$. With different actual heads under similar pressure as the density of the mixed fluid changes, it is not convenient to describe the flow of variable-density fluids. So the two equations (1) and (2) are written with respect to equivalent freshwater head ψ instead of actual head (ϕ).

The D*(t) is assumed to be dependent to the travel time from a single input source and can be and can take arbitrary functional form. In this study, D*(t) is restricted to the following functions as given by Pickens and Grisak (1981b):

Constant

$$D^*(t) = D_o + D_m \tag{3}$$

Linear

$$D^*(t) = D_o \frac{t}{K} + D_m \tag{4}$$

Asymptotic

$$D^*(t) = D_o \frac{t}{t+K} + D_m \tag{5}$$

Exponential

$$D^*(t) = D_o \left[1 - \exp\left(-\frac{t}{K}\right)\right] + D_m \tag{6}$$

where D_o is the maximum dispersivity, D_m is the molecular diffusion, and K is equal to the mean travel time corresponding to $D_o + D_m$ for linear case, to $0.5D_o + D_m$ in the asymptotic case, and $0.632D_o + D_m$ for the exponential case.

BOUNDARY CONDITIONS

The boundary conditions for simulation of flow and solute transport through a leaky aquifer system are shown schematically in Fig. 1. A no-flow condition is imposed along the lower boundary. Recharge enters evenly along the upper boundary. The recharge distribution along the inflow boundary is time dependent. Along the right and left boundaries a constant pressure is maintained at the boundary nodes. At the bottom boundary, a no-flow of solute condition is considered. For the left boundary, a freshwater concentration is known. The right boundary is located at a point where the rate of change of concentration along it is equal to zero. At the top boundary a freshwater concentration are specified if the water table is higher the piezometric head, otherwise the rate of change of concentration in vertical direction is equal to zero.

The finite difference mesh is used to discretize a representative cross section of the aquifer. The domain is divided uniformly using 867 nodes with 17 nodes in the vertical direction and 51 nodes at the horizontal one. Using this descretization, we have $\Delta x = 4$m and $\Delta y = 2.5$m.

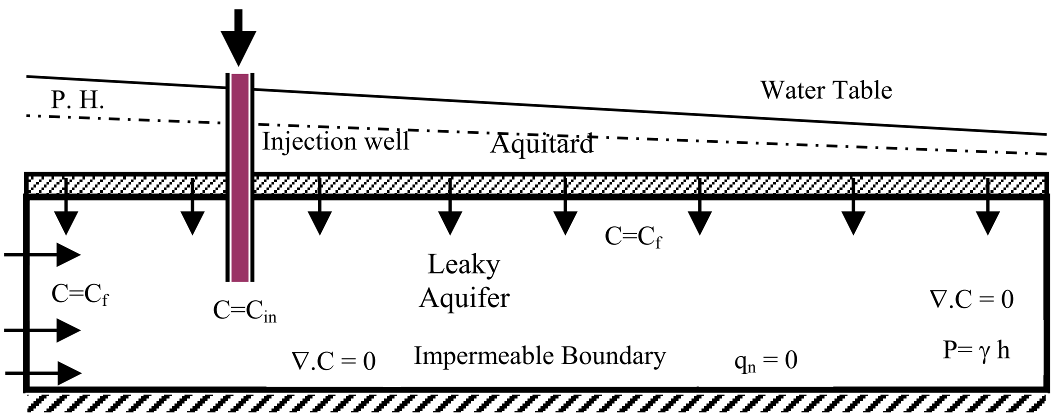

Figure 1: Boundary conditions

The flow equation is taken to satisfy the following initial and boundary conditions:

$$\psi(x_i,0) = \psi_o(x_i) \tag{7}$$

$$\psi(x_i,t)\left|B_1 = \psi^*(x_i,t)\right. \tag{8}$$

$$v_i n_i \left|B_2 = -v_n(x_i,t)\right. \tag{9}$$

where ψ_o is the initial head, ψ^* is the prescribed head on the Dirichlet boundaries B_1, $n=(n_1,n_2)$ is the outward unit vector normal to Neumann boundaries B_2, V_n is the prescribed lateral flow rate per unit area on B_2 (V_n is positive for inflow and negative for outflow). When B_2 is an impervious boundary and V_n is equal to zero.

$$v_i n_i \left|B_2 = 0\right. \tag{10}$$

The transport equation is taken to satisfy initial and boundary conditions:

$$C(x_i,0) = C_o(x_i) \tag{11}$$

$$C(x_i,t)\left|B_3 = C^*(x_i,t)\right. \tag{12}$$

$$D_{ij}\frac{\partial C}{\partial t} n_i \left|B_4 = 0\right. \tag{13}$$

where C_o is the initial concentration, C^* is the prescribed concentration on the Dirichlet boundaries B_3 and B_4 are impervious boundaries.

Eqs. (1) and (2), together with the relevant initial and boundary conditions are composed into a complete two-dimensional mathematical model for the description of solute migration in groundwater aquifers.

NUMERICAL SOLUTION

Eqs. (1) and (2) are nonlinear equations and they are solved numerically using central finite difference method, and they can be written finally in the following matrix form:

$$\left[G_\psi\right]\{\psi\} = \{A\} \tag{14}$$

$$\left[G_C\right]\{C\} = \{B\} \tag{15}$$

where, $[G_\psi]$ and $[G_C]$ are the coefficient matrices for the equivalent freshwater head and concentration, respectively. $\{\psi\}$ and $\{C\}$ are the unknown equivalent freshwater heads and concentrations, respectively, and $\{A\}$ and $\{B\}$ are known vectors containing the effect of boundaries.

MODEL APPLICATIONS

The model is applied for a leaky aquifer system subjected to continuous injection of solute through a well for three different scenarios. The first one for constant dispersion coefficient (K=0), second for time-dependent dispersion according to asymptotic form for a specified value of K and the last for another value of K. The aquifer dimensions are 200m length and 40m depth. The boundary conditions are shown in Fig. 1.

The left boundary is subjected to constant and equal to freshwater concentration C_f, the bottom boundary of is impervious. At the right boundary the concentration gradient is zero and this boundary is subjected to hydrostatic pressure distribution. The upper boundary is a leaky boundary. A continuous injection of solute is located at a distance of 32m and 25m from the left and bottom boundaries, respectively. Density of injected flow, ρ_{in} is 1035.0 kg/m^3 and its concentration, C_{in} is equal to 50 kg/m^3. Below the well, the concentration is set equal to the input concentration C_{in}. Hydraulic conductivities in the x and z directions are set equal to 100 m/day and 20 m/day, respectively. Longitudinal and transversal dispersivities, α_L and α_T are taken 10m and 1.0m, respectively in case of constant dispersion. Initially, the concentration is assumed to be constant and equal to freshwater concentration at every node inside the aquifer.

RESULTS AND DISCUSSION

Three scenarios were considered to investigate solute migration with time-dependent dispersion coefficient. In the first scenario, K in the Asymptotic equation (Eq. 5), is taken to be zero, case of constant dispersion. In the second and the third scenarios, K is taken to 2500 and 5000, respectively. In all scenarios, all geometric, physical and transport parameters were maintained constant but dispersion coefficient was changed. Simulations are carried out for 1000, 2500, and 5000 days after the beginning of the continuous injections. Figs. 2, 3, and 4 present equiconcentration lines for the different three scenarios, respectively.

In Fig. 2, case of constant dispersion coefficient, equiconcentration line 0.3 of the input concentration advanced a distance of 59m, 80m, and 110m measured from the left boundary after 1000, 2500, and 5000 days respectively. Equiconcentration line 0.1 advanced a distance of 78m and 109m after 1000 and 2500days, respectively. After 5000days, equiconcentration line 0.1 advanced to a distance of 154m and intersected the bottom boundary at a distance of 70m as shown in Fig. 2c.

Figure 3 represents the model results when the time-dependent approach is applied. All hydraulic parameters and geometric dimension are kept constant except K value is taken to be 2500. Equiconcentration line 0.1 advanced a distance of about 68m, 100m, and 145m while equiconcentration line 0.3 advanced a distance of 52m, 81m, and 117m, measured from the left boundary after 1000, 2500, and 5000days, respectively. When K value is taken to be 5000, equiconcentration line 0.1 advanced a distance of about 67m, 98m, and 148m while equiconcentration line 0.3 advanced a distance of 53m, 82m, and 120m after 1000, 2500, and 5000days, respectively as shown in Figs. 4a, b, and c.

It is noticed that the width of the dispersion zone for increases in the case of constant dispersion coefficient and occupied a larger area than the case of time-dependent dispersion. But the higher equiconcentration lines advanced to a distance larger than that of the case of constant dispersion.

All model results are summarized in Fig.5. It shows the advance of the concentration profile for a continuous injection at fixed locations. In the figure, the breakthrough curves at two locations (8m and 24m measured from the injection well) for various values of K are shown. It is clearly show the dependence of concentration profile on the value of K at early time. It is noticed that the effect of K on the slope of the concentration time curve. The family of curves shown in Fig. 5 could be considered to interpret tracer tests.

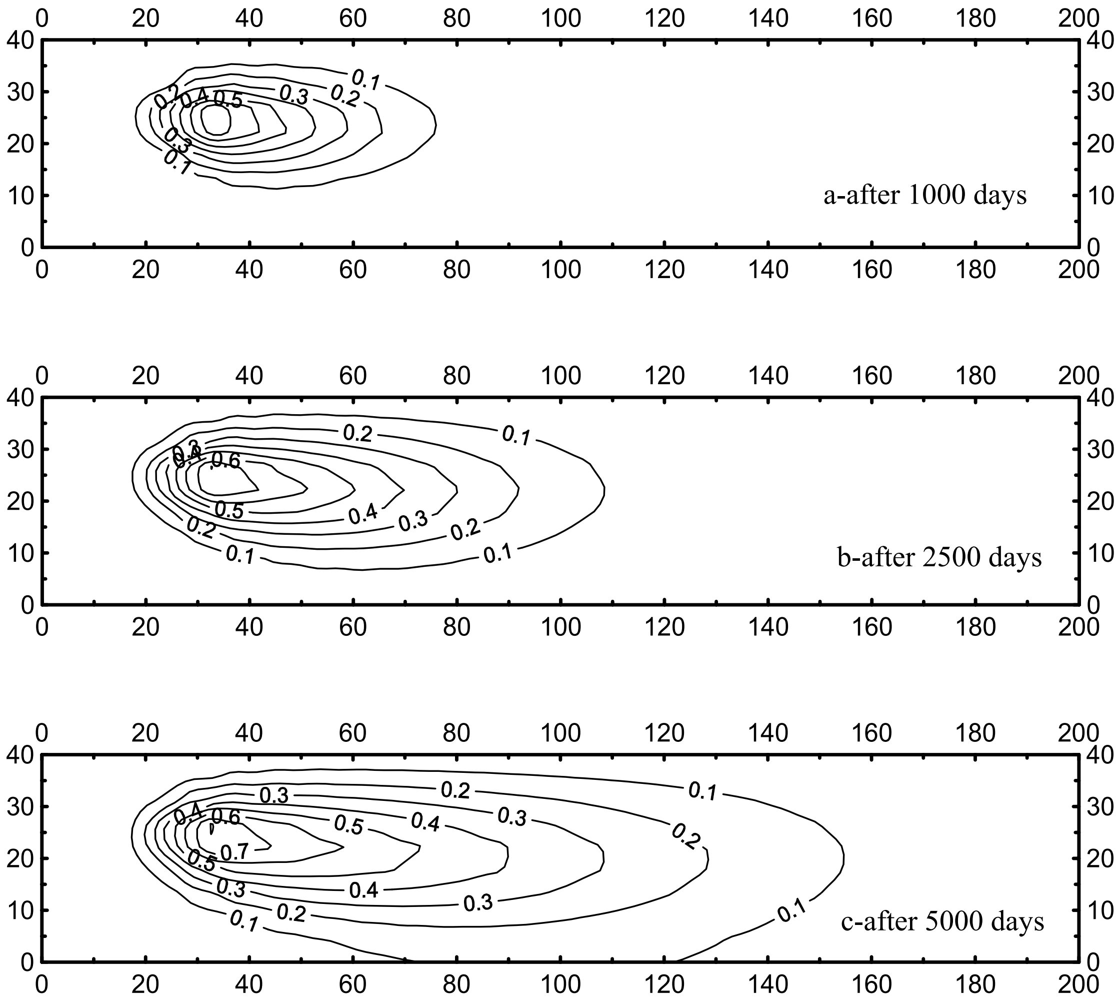

Figure 3: Equiconcentration lines for constant dispersion coefficient (Basic run)

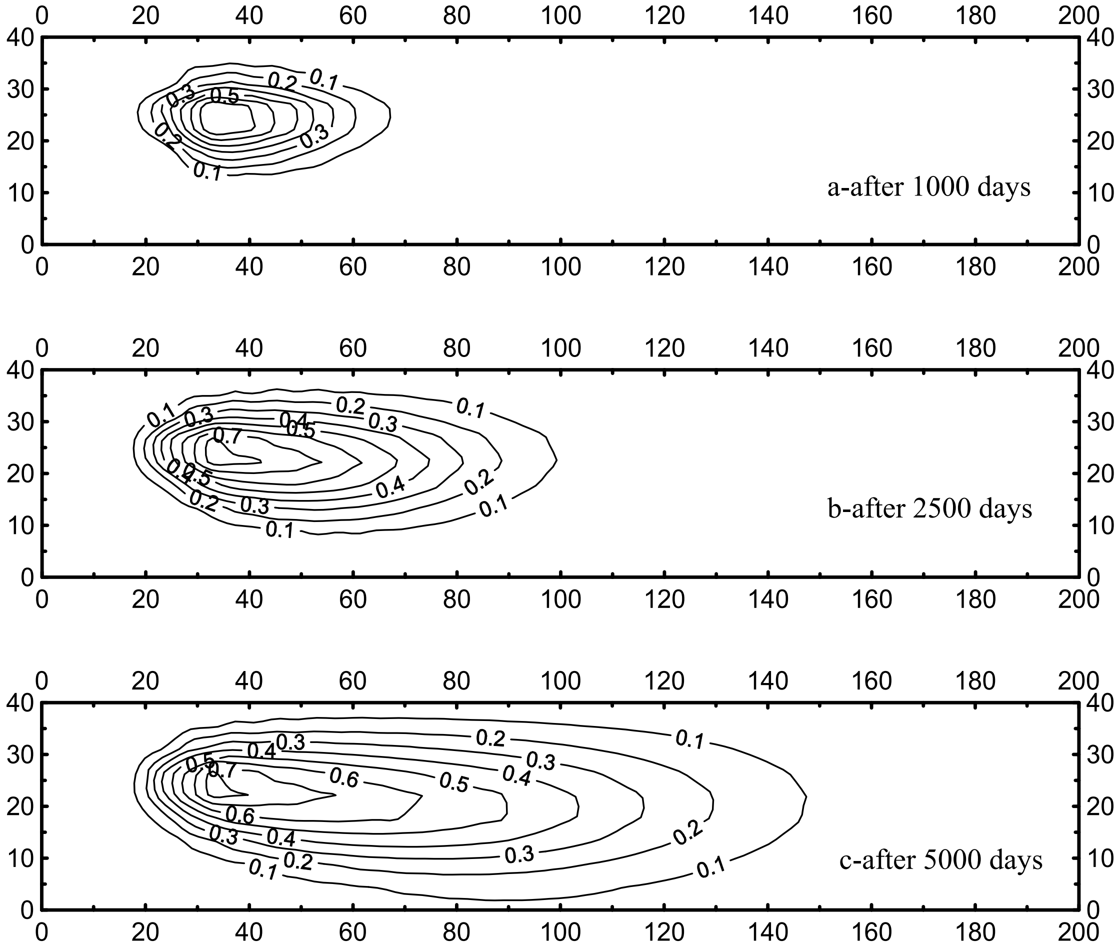

Figure 4: Equiconcentration lines for time-dependent dispersion coefficient with K = 2500

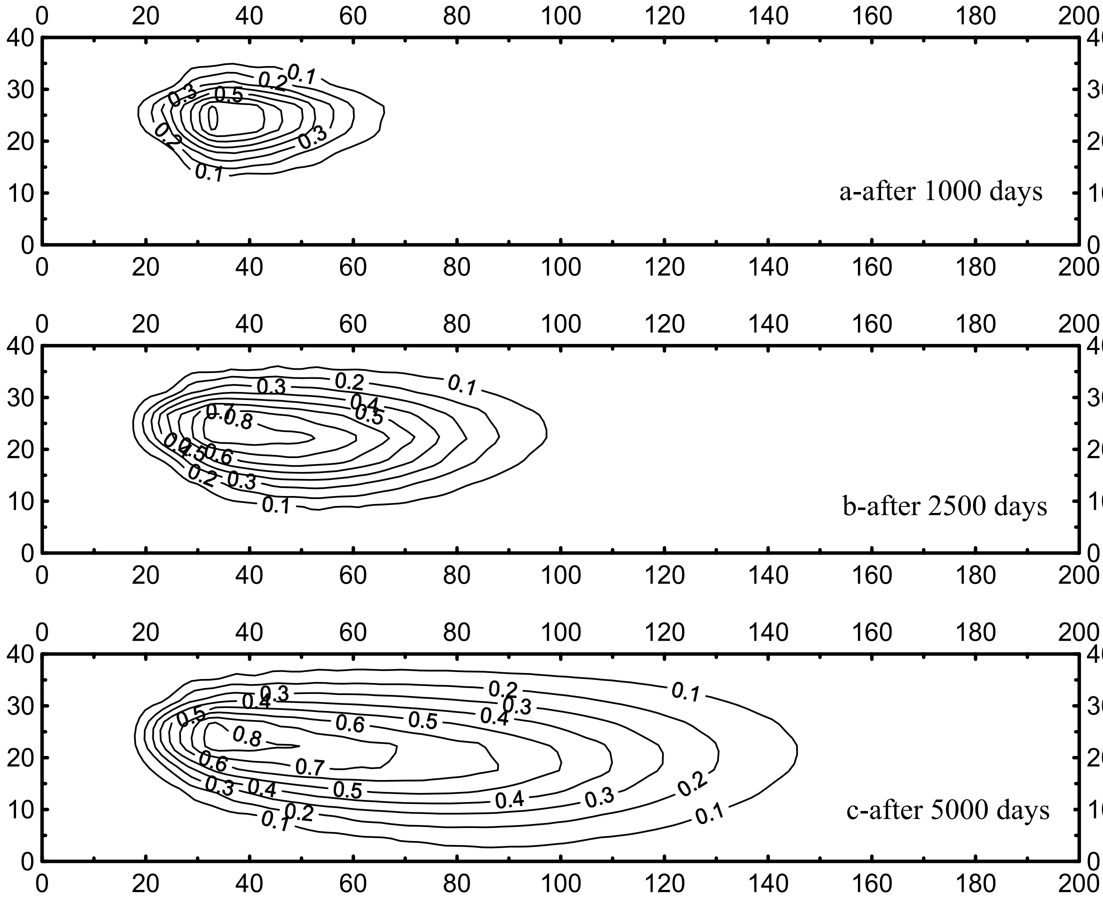

Figure 5: Equiconcentration lines for time-dependent dispersion coefficient with K = 5000

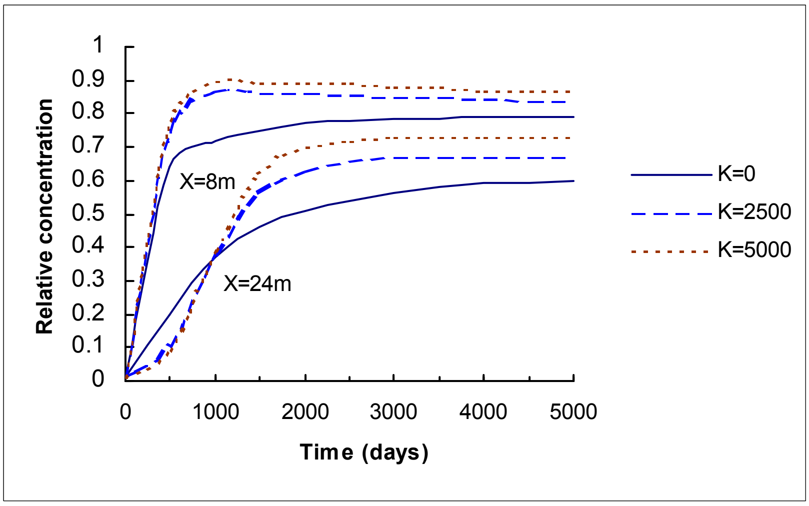

Figure 6: Breakthrough curves for various values of K.

CONCLUSIONS

The main purpose of this paper was to derive a solution to a convection-dispersion equation with time-dependent coefficients in a semi-infinite domain. The analysis is restricted to the asymptotic dispersion function since it is of more practical importance. The numerical solution with time-varying mass injection in a leaky aquifer system was presented. The density-dependent approach was used. It is assume that the flow is two-dimensional with variable velocity depending on the equivalent freshwater head with a single source of pollution. A comparison between the classical equation ($K=0$) and the model described herein ($K\neq0$) show that there is a significant difference in the concentration distribution during the early travel time in a scale-dependent hydrologic system. Using the time-dependent dispersion model described herein could be an alternative mean for obtaining aquifer dispersion parameters for situations where the dispersion coefficients are not constant. These numerical results could be useful for screening purposes if data are uncertain and provides a better solution than the classical constant dispersion model in hydrogeologic formations that exhibit a scale effect.

References

Basha, H.A. and El-Habel, F.S., "Analytical solution of the one-dimensional time-dependent transport equation," *Water Resour. Res.*, **29**(9): 3209-3214, 1993.

Barry, D.A., and Sposito, G.," Analytical solution of a convection-dispersion model with time-dependent transport coefficients," *Water Resour. Res.*, **25**: 2407-2416, 1989.

Cannon, J.R.," *The one-dimensional Heat Equation*, Addison Wesley, Reading, Mass, 1984.

Gelhar L.W., Lutjahr, A.L., and Naff, R.L., " Stochastic analysis of macrodispersion in a stratified aquifer," *Water Resour. Res.*, **15**: 1387-1397, 1979.

Güven, O., Molz, F.L., and Melville, J.G., " An analysis of dispersion in a stratified aquifer," *Water Resour. Res.*, **20**: 1337-1354, 1984.

Hamza, K.I., "A scale-dependent dispersion in porous media," In: Proc. Int. Conf. on Geoenvironment, eds. A. El-Zawahry, et al., pp. 478-486, Muscat, 2000.

Peckens, J.F. and Grisak, G.E., "Scale-dependent dispersion in a stratified granular aquifer," *Water Resour. Res.*, **17**: 1191-1211, 1981a.

Peckens, J.F. and Grisak, G.E., "Modeling of scale-dependent dispersion in hydrogeologic systems," *Water Resour. Res.*, **17**: 1701-1711, 1981b.

Sauty, J.P., " An analysis of hydrodispersive transfer in aquifers," *Water Resour. Res.*, **16**: 145-158, 1980.

Serrano, S.E., " The form of the dispersion equation under recharge and variable velocity, and its analytical solution," *Water Resour. Res.*, **28**: 1801-1808, 1992.

Sposito, G., Jury, W. and Gupta V.K., "Fundamental problems in the stochastic convection-dispersion model of solute transport in aquifers and field soils," *Water Resour. Res.*, **22**(1), 77-88, 1986.

Spositto, G., and Barry, D.A.,“On the Dagan model of solute transport in groundwater: Fundamental aspects, ” *Water Resour. Res.*, **23**(10), 77-88, 1987.

Yates, S.R., “ An analytical solution for one-dimensional transport in heterogeneous porous media,” *Water Resour. Res*., **26**: 2331-2338, 1990.

Yates, S.R., “ An analytical solution for one-dimensional transport in porous media with exponential dispersion function,” *Water Resour. Res*., **28**: 2149-2154, 1992.

Keywords: Time-dependent, dispersion, asymptotic, variable density

Corresponding author: Khaled Ismail Hamza, Associated Professor of Civil Engineering, Faculty of Engineering, The Hashemite University, P.O. Box 150459, Postal Code, 13115, Zarqa, Jordan. Email: kihamza@hotmail.com