

A characteristic study of dispersion parameters for solute transport in groundwater

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Abstract

The present study is an attempt to evaluate the behaviour of constituents/pollutants moving with groundwater. Three examples using data of basic parameters from literature have been demonstrated. Dispersivity, adsorptivity and decay which are primary parameters affecting the transport phenomena have been considered. The dispersivity which is the main characterizing parameter in transport problems, have been considered for sensitivity analysis. It has also been attempted to quantify errors involved when a two/three-dimensional problem is simplified to a one-dimensional problem.

The result indicated that one-dimensional analytical and numerical solution of transport equation compare well –but- simplifying a two/three-dimensional transport problem to a one-dimensional problem leads to error due to transverse dispersion. Close to the source, advection dominates whereas away from it the dispersion phenomena dominates. It was also seen that transverse dispersivity becomes prominent as distance increases from the source.

INTRODUCTION

Groundwater is a source for fresh drinking water besides its use in industrial, agricultural and other domestic uses. During recent times due to over use and abuse of groundwater resources, the stresses imposed on the groundwater system have increased steadily. Not only its quantitative over exploitation have occurred, but also a qualitative assault on groundwater bodies have taken place. This has resulted in depletion of groundwater resources. Once contaminants from the unsaturated zone containing dissolved constituents move to the saturated zone, it is transported due to groundwater flow and disperses in all possible directions.

Contaminant's transport in groundwater is largely governed by the parameters which shapes the groundwater flow equation. In addition, it is also governed by factors like: i) advection of the constituent with the water flowing through the aquifer, ii) dispersion of the constituent, iii) addition/removal of the constituent to/from the system, and iv) chemical reaction. Therefore, to simulate contaminant transport phenomena, first it is necessary to simulate groundwater flow.

Numerous analytical and numerical models are available to simulate flow and transport phenomena in a groundwater system. The basic concept of solving flow and transport equation is the mass-balance equation. Analytical models can be used for solving

groundwater flow and transport equation with simple initial and boundary conditions. But, analytical methods in most cases cannot represent real field situation because of heterogeneity of aquifer parameters, irregular shape of the domain boundaries and temporal, spatial distributions of the various sink-sources functions etc.

Common problems in groundwater transport modelling is the absence of direct means for determination of dispersivity in the field, lack of knowledge of exact chemical reactions occurring during movement of constituents etc. To simplify the flow and transport problems, the most common assumptions are : i) consideration of one-dimensional flow and transport, ii) constituents are assumed to have same properties and their decay and absorption/adsorption rate are constant. These simplifications lead to a wide disagreement between observed and computed values of groundwater head and concentration.

PRESENT STUDY AND OBJECTIVES

The present study is an attempt to evaluate the behaviour of constituents/pollutants moving with groundwater. Three examples keeping relevance to field conditions have been demonstrated in the study. Dispersivity, adsorptivity and decay affecting the transport phenomena have been considered. The sensitivity of parameter mainly dispersivity characterising the transport problems, have been analysed. Attempts have also been made to quantify errors when a 3-D problem is simplified to a 2-D problem and a 2-D problem to a 1-D problem.

The first case example deals with a simple *one-dimensional* transport problem involving advection, dispersion, adsorption and decay. The problem is solved by analytical method. Results obtained from it is compared with the result obtained from well known numerical flow/transport model MODFLOW/MT3D to quantify the disagreement in solutions. Later, the same problem is extended to a *two-dimensional* case, and the effect of transverse dispersivity is considered. This is to evaluate the quantum of deviation in the concentration profile as compared to the result obtained in one-dimensional case.

The second case example is a *two-dimensional* case with a source and sink situation. Contaminant is injected into the aquifer through an injection well for a given time is considered as source, and pumped out from the same well is considered as sink. The sensitivity of longitudinal and transverse dispersivities on the concentration profile in time and space have been studied by assigning different values of dispersivities.

The third case example deals with a *three-dimensional* transport of pollutant from a waste dump site. The migration of pollutant is analyzed by assuming different longitudinal and transverse (both horizontal and vertical) dispersivities. Here, the aim is to see the effect of transverse dispersivities on the concentration profile both in space and time. It is also envisaged to see whether transverse dispersivity dominates over the longitudinal dispersivity beyond a certain distance from the source of the waste dump site.

MATHEMATICAL BACKGROUND

The three dimensional unsteady movement of groundwater of constant density through porous earth material in a heterogenous anisotropic medium can be described by the following partial differential equation:

$$\frac{\partial}{\partial x} \left(K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t} \quad (1)$$

Where, K_{xx} , K_{yy} , K_{zz} = hydraulic conductivity along major axes [LT^{-1}]; h = potentiometric head [L]; W = volumetric flux per unit volume and represents sources and/or sinks of water [T^{-1}]; S_s = specific storage of the porous material [L^{-1}] and t = time [T].

A mathematical model for the transport of solute in groundwater can be derived by taking the mass balance of the dissolved pollutant over a static elementary volume. Expressed in words the equation can be written as:

Change in solute mass *stored* =
excess solute mass *diffusion* into volume + excess solute mass inflow over outflow or mass transport by *Convection and Dispersion* + solute mass added by *injection/infiltration* - solute mass lost by *withdrawal* - solute mass lost by *decay* - solute mass lost by *reaction* - solute mass *adsorbed* on solid interface.

Mathematically, the above transport equation is expressed as:

$$\begin{aligned} \frac{\partial(nc)}{\partial t} = & \frac{\partial}{\partial x_i} \left(nD_m \frac{\partial c}{\partial x_i} \right) - \frac{\partial}{\partial x_i} (nv_i c) + \frac{\partial}{\partial x_i} \left(nD_{ij} \frac{\partial c}{\partial x_j} \right) + q_{3i} c_i - q_{3a} c \\ & - n \lambda_c c - n \zeta_c - \left[\frac{\partial}{\partial t} \left((1-n) \rho_s c_a \right) + \lambda_a (1-n) \rho_s c_a + (1-n) \zeta_a \right] \end{aligned} \quad (2)$$

Where, n = porosity[-]; c = concentration of dissolved pollutants [ML^{-3}]; t = time [T]; x_i = distance tensor [L] (subscript $i = 1,2,3$. $x_1 = x$; $x_2 = y$; $x_3 = z$); D_m = coefficient of molecular diffusion [L^2T^{-1}]; v_i = velocity tensor [LT^{-1}]; D_{ij} = coefficient of dispersion tensor [L^2T^{-1}] (when $i=1=x$; $i=2=y$; $i=3=z$ and when, $j=1=x$; $j=2=y$; $j=3=z$); q_{3i} = volumetric infiltration (+ = infiltration) [T^{-1}]; c_i = concentration of pollutant in infiltrated water [ML^{-3}]; q_{3a} = volumetric abstraction (+ = abstraction) [T^{-1}]; λ_c = decay constant for dissolved pollutants [T^{-1}]; ζ_c = volumetric reaction rate of dissolved pollutants [$ML^{-3}T^{-1}$]; λ_a = decay constant for adsorbed pollutants [T^{-1}]; ρ_s = density of solids (grains) [ML^{-3}]; c_a = concentration of adsorbed pollutants [MM^{-1}]; ζ_a = volumetric reaction rate of adsorbed pollutants [$ML^{-3}T^{-1}$].

Equation (2) is the governing equation underlying a solute transport model. The transport equation and the flow equation is linked through the relationship:

$$v_i = -\frac{K_{ii}}{n} \frac{\partial h}{\partial x_i} \quad (3)$$

Where, K_{ii} = principal component of hydraulic conductivity tensor, $[LT^{-1}]$; h = hydraulic head[L].

In the present study, numerical transport model MT3D (Chunmiao Zheng, 1990) compatible with flow model MODFLOW (Mc Donald and Harbough, 1988) have been used to solve above flow and transport equations.

3-dimensional solute transport equation (2) when reduced to *1-dimensional form* (Ogatta and Banks 1961) under assumptions of i) constant porosity; ii) constant aquifer thickness; iii) convective velocity 'v' is constant (i.e steady state groundwater flow); iv) since 'v' is constant and $D = \alpha_L |v|$, therefore, 'D' is also constant; v) molecular diffusion is very very small i.e. diffusion may be neglected; vi) no decay; and vii) no reaction, becomes:

$$c(x,t) = \frac{I}{2} c_o \operatorname{erfc} \left[\frac{x - \frac{v}{R} t}{2 \sqrt{\alpha_L \frac{|v|}{R} t}} \right] \quad (4)$$

Where, c_o = initial concentration of dissolved pollutants $[ML^{-3}]$; 'erfc' is the complementary error function; x = distance in x-direction[L]; R = retardation factor[-]; α_L = longitudinal dispersivity[L]; $|v|$ = magnitude of local groundwater velocity $[LT^{-1}]$; α_T = transversal dispersivity[L]

CASE STUDIES

1-D, 2-D Case Problem

One-dimensional steady state flow domain consists of 100 columns, 1 row and 1 layer. The input parameters for flow and transport simulation are :

For flow:

Cell width along rows (Δx)	= 25m.
Cell width along column (Δy)	= 25m.
Layer thickness (Δz)	= 25m.
Aquifer type	= unconfined.
Porosity (n)	= 0.25.
Homogenous hydraulic conductivity (k)	= 40m/day.
Constant head cell at (1,1) and (100,1) with head	= 70m and 60 m respectively.

No external stresses (viz. well, drains, river, evapotranspiration, aerial recharge, stream aquifer relation) considered.

For transport:

The cell in the first column (1,1) is treated as a constant concentration cell with concentration = 1 kg/cum.

Starting concentration at all other cell = 0 kg/cum.

Longitudinal dispersivity (α_L) = 20m, Retardation factor (R) = 5 and Decay or the rate constant of the first order rate reaction (λ) = 0.002 day⁻¹.

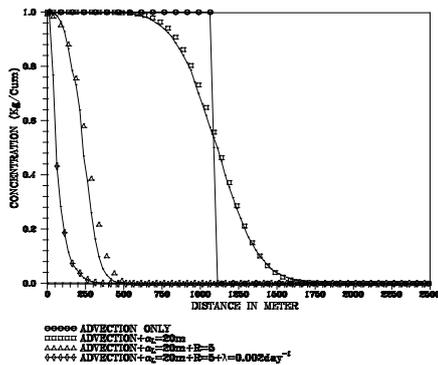


Figure 1. Effect of Advection, Dispersion, Adsorption and Decay on the Concentration Profile in an 1-D Problem (line \Rightarrow Numerical solution and point \Rightarrow Analytical solution).

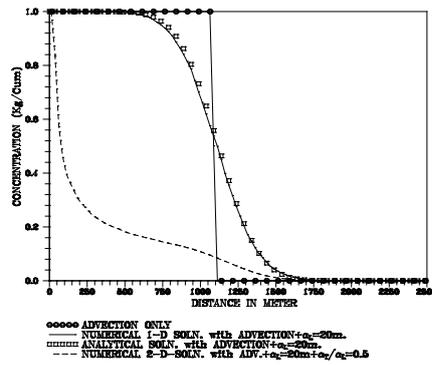


Figure 2. Comparison of Advection + Dispersion on the Concentration Profile in a 1-D and 2-D Problem (line \Rightarrow Numerical 1-D solution and dashed line \Rightarrow 2-D solution).

First, the 1-D transport problem involving advection; advection + dispersion; advection + dispersion + adsorption; and advection + dispersion + adsorption + decay are solved separately by analytical procedure (eqⁿ 4) suggested by Ogata and Banks (1961). In this problem, only the *longitudinal dispersivity* is considered. The same problem is also solved numerically using MT3D model. Comparison of results are given in Figure 1.

The result (concentration v/s distance) shows an excellent match between the analytical and numerical solution which eventually show that the 1-D transport phenomena can well be represented by the 1-D model.

Next, the same example is extended to a 2-D case with 100 X 100 grids. The first and the last column is assumed to be constant head cells for flow simulation. For simulation of constituent's transport, only Cell (1,51) is assumed to be a constant concentration cell. The transverse dispersivity is assumed to be half the longitudinal dispersivity. All other parameters of flow and transport are kept same. In fact, a real field problem involves spreading of pollutant concentration in all directions. These spreading reduces the concentration at a point as compared to a 1-D problem. The simulated results (concentration profile) advocating the effect of advection + dispersion in a 2-D test case is shown in Figure 2. The results of the 1-D case for advection + dispersion is also shown in the same figure for comparison.

The results indicate an appreciable deviation in concentration along 51st row as compared to 1-D case. This difference (reduction) in concentration is due to spreading of pollutants along the transverse direction. This demonstrates the quantum of errors involved when a 2-D or even a 3-D problem is simplified to a 1-D problem.

Similar nature of concentration profiles have also been seen from the result of simulation involving advection + dispersion + adsorption; and advection + dispersion + adsorption + decay.

Injection/Pumping Well Problem

A fully penetrating well in a confined aquifer is used for studying the transport behaviour of pollutant injected through it and later the same well is used for extraction/sweeping of the contaminants. A pollutant of constant concentration is injected through the well during the first stress period. During the next stressed period, the flow is reversed and the contaminated water is pumped out. The effect of variation of input value of *longitudinal dispersivity* on the simulated concentration v/s time profiles in these two stress periods at various distances from the injection/pumping well is seen.

The transient 2-D injection/pumping problem taken for analysis consist of 51 rows, 51 columns and 1 layer with a well located at the centre of the area in the cell (26,26). The input data for flow and transport simulation are as follows:

For flow:

1st stress period (Injection)	= 910 days \approx 2.5 years.
2nd stress period (Pumping)	= 2740 days \approx 7.5 years.
Cell width along rows (Δx)	= 100m.
Cell width along column (Δy)	= 100m.
Layer thickness (Δz)	= 20m.
(Top RL = 100m and Bottom RL = 80m.) Aquifer type	= Confined.
Porosity (n)	= 0.30
Homogenous hydraulic conductivity (k)	= 50m/day.
Constant head cell at four sides of the boundary.	
Injection rate	= 2500cum/day.
Pumping rate	= 2500cum/day.
Other external stresses are ignored.	

For transport:

All cells are considered as variable concentration cell with starting concentration as zero.

In the well package, concentration of the injected water is taken as = 100g/cum.

Advective and Dispersive transport is assumed. No chemical reaction is considered.

Longitudinal dispersivity (α_L) considered = 10m, 50m and 75m.

Model is also simulated for $\alpha_T/\alpha_L = 1$ i.e Transversal dispersivity and Longitudinal dispersivity are same.

Observation points are chosen at the well and at 100m, 300m and 500m from the well.

Results of flow simulation reveals that during the injection period, the flow is out of the well towards the boundary sides, and during pumping period, the flow is towards the well.

After simulation of flow, transport model is run initially with advective transport, and afterwards with different values of longitudinal dispersivity. To examine the effect of transverse dispersivity on the concentration profile, transverse dispersivity is considered to be equal to the longitudinal dispersivity (i.e $\alpha_T/\alpha_L = 1.0$) and the model is simulated. The breakthrough curves (time-concentration profile) at different observation points located at specified distances from the well is plotted for different values of longitudinal dispersivity and for $\alpha_T/\alpha_L = 1.0$ (Figure 3 to 6).

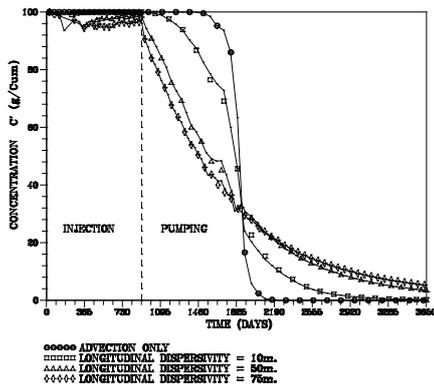


Figure 3. Breakthrough curves at the well with Advection and different values of Longitudinal Dispersivity (line \Rightarrow with Longitudinal dispersivity; symbols $\Rightarrow \alpha_T/\alpha_L = 1.0$).

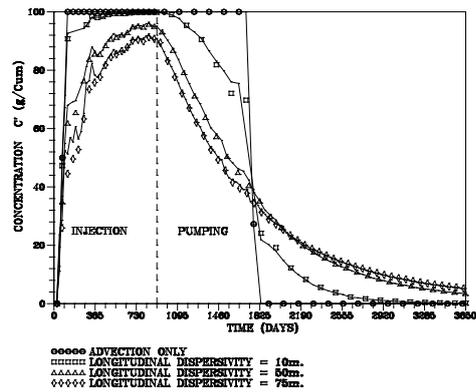


Figure 4. Breakthrough curves at 100m from the well with Advection and different values of Longitudinal Dispersivity (line \Rightarrow with Longitudinal dispersivity; symbols $\Rightarrow \alpha_T/\alpha_L = 1.0$).

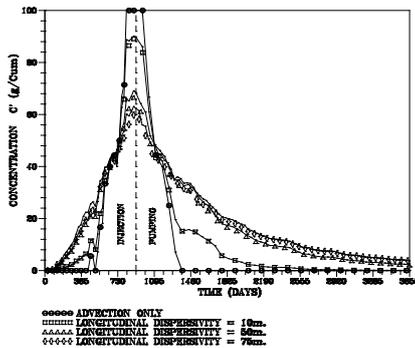


Figure 5. Breakthrough curves at 300m from the well with Advection and different values of Longitudinal Dispersivity (line \Rightarrow with Longitudinal dispersivity; symbols $\Rightarrow \alpha_T/\alpha_L = 1.0$).

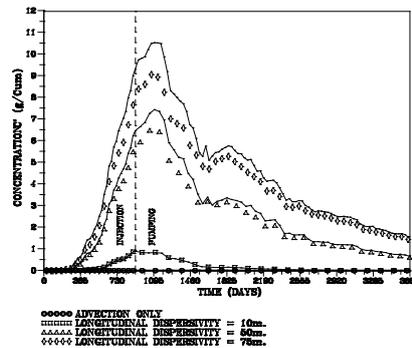


Figure 6. Breakthrough curves at 500m from the well with Advection and different values of Longitudinal Dispersivity (line \Rightarrow with Longitudinal dispersivity; symbols $\Rightarrow \alpha_T/\alpha_L = 1.0$).

From these figures, it is evident that concentration profiles show differences away from the well. This leads one to draw the following inferences:

With increase in value of the longitudinal dispersivity, reduction of concentration of constituents occurs upto a certain distance from the well (upto 300m in the present case) as is apparent from Figure 5.

For larger value of dispersivity, the fall of concentration during the pumping cycle is gradual i.e the concentration reduces at a slower rate for larger value of dispersivity. Thus, concentration profile extends for a longer period for higher value of dispersivity.

The effect of transverse dispersivity, when $\alpha_T/\alpha_L = 1.0$, becomes significant at a longer distance from the well. In the case example it started becoming apparent at 300m from the well as seen in Figure 5. In the closer proximity of the well, the difference in the effect of longitudinal dispersivity and transverse dispersivity is insignificant.

Closer to the well, the influence of advective transport is dominant and the influence decreases with increase in distance from the well and for larger distance it becomes insignificant. Beyond certain distance from the well (in the example case from a distance of 500m from the well), the dispersion phenomena dominates and the concentration profile shows a reversal of trend in concentration profile i.e more the longitudinal dispersivity, more is the concentration. This can well be explained from Figure 6.

Dominancy of dispersive transport over the advective transport shifts the peak of concentration profile (Figure 6).

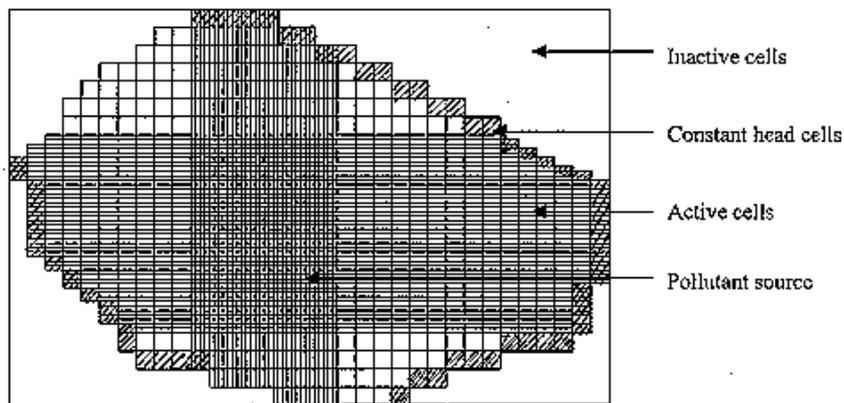


Figure 7. Gridal network of 3-D model area (number of cells in X-direction = 57 and number of cells in Y-direction = 55).

3-D Waste Dump Problem

To study the behaviour of constituent's transport in 3-dimension, a hypothetical study area as shown in Figure 7 is considered. It is assumed that a deposit of Benzene in dissolved form lies in the central part of the area covering cells shown in Figure 7. The pollutant in dissolved form enters the aquifer system with a concentration equal to 0.0001

kg/cum. Assuming a steady state condition of flow for the area with the following input data and boundary conditions, the time-concentration profile at a number of observation points located at different distances from the dump site for 20 years after beginning of benzene migration in the aquifer is analyzed.

The aquifer is assumed to have two layers confined in nature. The model area is discretized into 55 rows and 57 columns as shown in Figure 7. The boundaries of the model area in the north-east, east, south-east and south-west sides are defined by canal which are in full hydraulic contact with the aquifer. They are treated as fixed head boundaries. Other boundaries are defined by streamlines and are therefore impervious (no-flow boundaries). The input data, aquifer parameters and solute properties are assumed constant everywhere as defined below:

For flow:

Thickness of the first aquifer	=	8m.
Thickness of the second aquifer	=	7m.
Cell width along rows and columns	=	100m, 25m and 100m.
Porosity (n)	=	0.2.
Horizontal hydraulic conductivity	=	50m/day.
Vertical hydraulic conductivity	=	1/20 of Hoz. hydraulic conductivity.
Aerial recharge	=	0.00216 m/day.

For transport:

All cells in the model area are considered as variable concentration cells.
Concentration of pollutants = 0.0001 kg/cum entering with the recharge water.
Advection, dispersion and chemical reactions have been assumed.
Longitudinal dispersivity (α_L) = 5m, 10m and 20m.
The ratio of horizontal and vertical transverse to longitudinal dispersivity = 0.5
Distribution coefficient (k_d) of Benzene = 0.0002 cum/kg.
Bulk density of the porous medium in the aquifer = 1700 kg/cum.

The flow is simulated assuming steady state condition. The computed isolines indicate an outflow towards the south-western side i.e towards canal boundaries. To demonstrate the transport behaviour, two observation points at cells (22,35) and (18,39) are chosen in both layers of the aquifer.

Responses of concentrations at cell (22,35) over different time are shown in Figures 8 and 9 which reveals that:

Increase in longitudinal dispersivity decreases the concentration.
Combined effect of longitudinal and transverse (horizontal and vertical) dispersivity reduces the concentration further.
In the first aquifer where the dump site is located, the spread of pollutant influence both by the longitudinal and transverse (horizontal and vertical) dispersivities.
In the second layer the occurrence of pollutant concentration is dominated by the combined effect of longitudinal and transverse dispersivity. The effect of longitudinal disper-

sivity alone, is negligible. Away from this cell, similar trend could also be seen excepting that concentration reduces with increase of distance from the dump site.

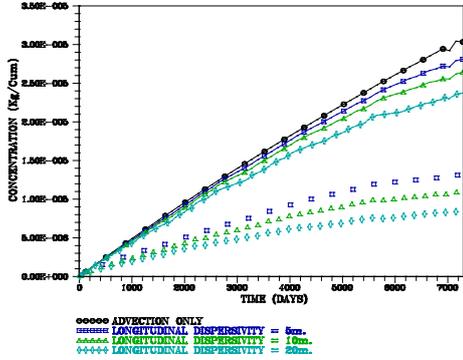


Figure 8. Breakthrough curves at cell (22,35) for the first layer with advection and with different values of dispersivities (line with symbols \Rightarrow with longitudinal dispersivity; only corresponding symbols $\Rightarrow \alpha_T/\alpha_L = 0.5$ and $\alpha_V/\alpha_L = 0.5$).

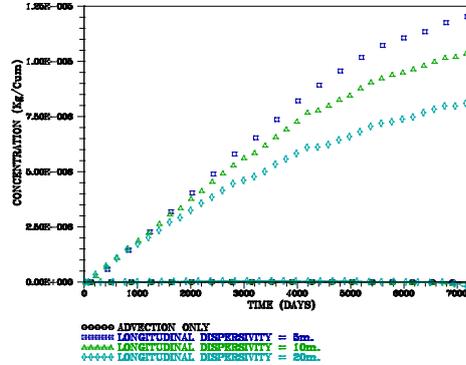


Figure 9. Breakthrough curves at cell (22,35) for the 2nd layer with advection and with different values of dispersivities (line with symbols \Rightarrow with longitudinal dispersivity; only corresponding symbols $\Rightarrow \alpha_T/\alpha_L = 0.5$ and $\alpha_V/\alpha_L = 0.5$).

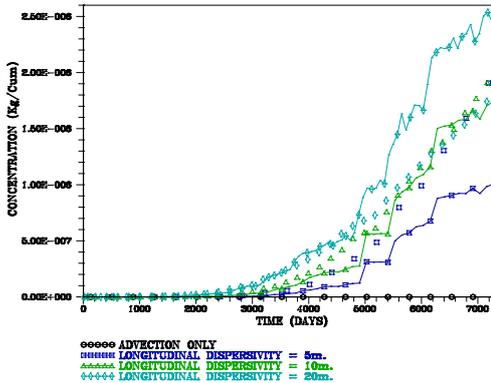


Figure 10. Breakthrough curves at cell (18,39) for the first layer with advection and with different values of dispersivities (line with symbols \Rightarrow with longitudinal dispersivity; only corresponding symbols $\Rightarrow \alpha_T/\alpha_L = 0.5$ and $\alpha_V/\alpha_L = 0.5$).

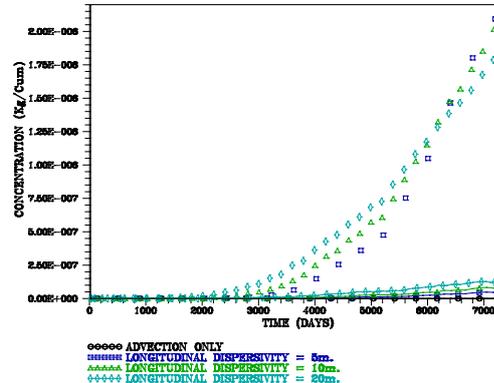


Figure 11. Breakthrough curves at cell (18,39) for the 2nd layer with advection and with different values of dispersivities (line with symbols \Rightarrow with longitudinal dispersivity; only corresponding symbols $\Rightarrow \alpha_T/\alpha_L = 0.5$ and $\alpha_V/\alpha_L = 0.5$).

A reverse trend is observed for cell (18,39) shown in Figure 10 in the first layer. In this case, the concentration due to advective transport becomes negligible and with increase in dispersivities, the concentration also increases. It means - the occurrence of pollutant at a farther distance is influenced by the dispersion phenomena and the concentration is more for higher dispersivity. In the second layer also (Figure 11), similar trend is observed, i.e concentration is more due to the effect of horizontal and vertical transverse dispersivity and it is more for higher dispersivity.

CONCLUSIONS

One-dimensional analytical solution and results of numerical transport model compare well.

Simplification of a two or three-dimensional transport problem as one-dimensional will lead to errors due to transverse dispersion.

The effect of transverse dispersivity becomes prominent as distance increases from the source.

Close to the source, the advection dominates the transport phenomena, and its influence decreases with increase in distance from the source in the direction of groundwater flow.

When the distance from the source increases, dominancy of dispersive transport over the advective transport shifts the peak of concentration profile.

Combined effect of longitudinal and transverse dispersivity reduces the concentration further as compared to longitudinal dispersivity considered alone.

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