One and Two-dimensional Contaminant Transport Modelling through Unconfined Aquifer

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Abstract – *In this study, an effort is made to develop a finite difference model to predict the movement of contaminant in an unconfined aquifer, considering both one- and two-dimensional flow field conditions for movement. It includes advection dispersion equation for a given set of initial and boundary conditions because concentration of contaminants usually gets altered while moving with ground water due to the effect of mechanical dispersion, advection, adsorption and radioactive decay. The represented profile in all direction for 2D is useful to understand the intensity of damage to aquifer.*

Key Words: steady state, computational sophistication, contaminant plume, advection-dispersion, degradation, discretized domain

1.INTRODUCTION

Ground water, held in aquifer is reliable and safer for drinking in comparison with surface water. Due to increment in industries, availability of clean water in aquifers is under threat. The scarcity of drinking water already affecting many parts of India. For saving the life of common citizens, it is necessary to control and predict the movement of contaminant particles to reach the ground water resources. More than 60% of irrigated agriculture and 85% of drinking water supplies are dependent on groundwater (Gurganus, 1993). This by no means says that groundwater is safe to contamination. It generally has a high-quality standard in India but today different kinds of human impacts are increasingly contaminating the groundwater resources. Any chemicals that are easily soluble and penetrate the soil are prime candidates for groundwater pollutants. Once it is contaminated, it is extremely difficult and costly to remove the contaminants from groundwater (Gurganus, 1993). Therefore, efforts are often put on protective measures instead. In order to know if, and to what extent groundwater is endangered, knowledge of the changes in groundwater quality is needed.

The sources of groundwater pollution can be divided into four major groups: environmental, domestic, industrial and agricultural. All groundwater contains salts carried in solution, which are added to groundwater by rain water, irrigation water, artificial recharge, soluble rock materials, fertilizers etc. Accidental breaking of sewers and percolation from the septic tank may also increase the pollution. When radioactive waste is deeply buried, there is a likelihood of groundwater getting contaminated (Gurganus, 1993).

There is a large amount of published material in the field of contaminant transport as-Guymon et al. (1970) and Nalluswami et al. (1972) used the finite element method (FEM) based on the variational principle for the solution of the dispersion problem in a rectilinear flow field. This method was found to be applicable to dispersion dominant transport only. Smith et al. (1973) compared the variational approach with the Galerkin method and concluding final more adaptable.

1.1 Governing Equations

For one-dimensional flow, the governing equation in a homogeneous, isotropic porous medium reduces to the familiar advection-dispersion equation (Bear 1972):

$$D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t} \quad (1.1)$$

While for two-dimensional flow with a direction of flow parallel to the x-axis, the equation becomes (Bear 1972):

$$\boldsymbol{D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial x^2} - v_x \frac{\partial c}{\partial x} - v_y \frac{\partial c}{\partial x} = \frac{\partial c}{\partial t}} \quad (1.2)$$

Where D_x is the longitudinal hydrodynamic dispersion coefficient.

D_y is the transverse hydrodynamic dispersion coefficient.

v_x is the advection velocity in the x-direction.

v_y is the advection velocity in y-direction.

C is the concentration of contaminants.

The current figure shows the discretized flow domain for 1-D advection-dispersion. Here i is the column number which represents the spatial discretization of the domain in the x-direction, j is the row number which represents the temporal discretization. Now one-dimensional advection-diffusion can be discretized by explicit method as –

$$\frac{\partial c}{\partial t} = \frac{c_i^{j+1} - c_i^j}{\Delta t} \tag{1.3}$$

$$\frac{\partial c}{\partial x} = \frac{c_{i+1}^j - c_i^j}{\Delta x} \tag{1.4}$$

$$\frac{\partial^2 c}{\partial x^2} = \left(\frac{c_{i+1}^j - 2c_i^j + c_{i+1}^j}{\Delta x^2}\right) \tag{1.5}$$

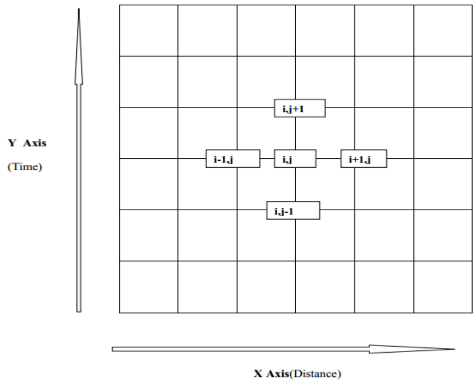

Fig. 1.1. Space and Time discretization for one-dimensional finite difference formulation

Putting Eqs. (1.3), (1.4) and (1.5) in Eq. (1.1), we get

$$C_i^{j+1} = C_i^j + \frac{D_x \Delta t}{(\Delta x)^2}\left(C_{i+1}^j - 2C_i^j + C_{i+1}^j\right) - \frac{v_x \Delta t}{\Delta x}\left(C_{i+1}^j - C_i^j\right) \tag{1.6}$$

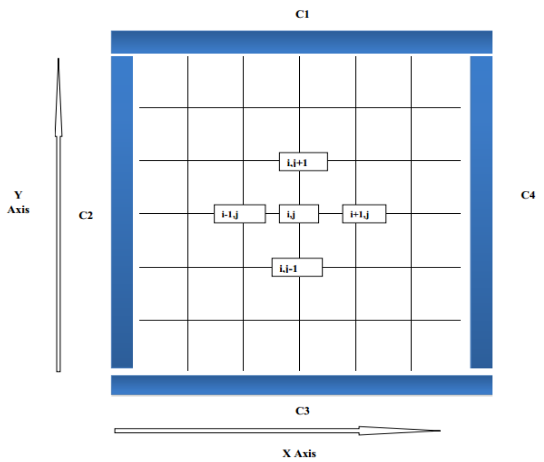

Fig. 1.2. Space and time discretization for two-dimensional finite difference formulation

$$\frac{\partial C}{\partial t} = \frac{C_{i,j}^{k+1} - C_{i,j}^k}{\Delta t} \tag{1.7}$$

$$\frac{\partial C}{\partial x} = \frac{C_{i+1,j}^k - C_{i,j}^k}{\Delta x} \tag{1.8}$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1,j}^k - 2C_{i,j}^k + C_{i-1,j}^k}{\Delta x^2} \tag{1.9}$$

$$\frac{\partial C}{\partial y} = \frac{C_{i,j+1}^k - C_{i,j}^k}{\Delta y} \tag{1.10}$$

$$\frac{\partial^2 C}{\partial y^2} = \frac{C_{i,j+1}^k - 2C_{i,j}^k + C_{i,j-1}^k}{\Delta y^2} \tag{1.11}$$

Putting all above expressions in equation (1.2)-

$$C_{i,j}^{k+1} = C_{i,j}^k + \frac{D_x \Delta t}{(\Delta x)^2}\left(C_{i+1,j}^k - 2C_{i,j}^k + C_{i-1,j}^k\right) + \frac{D_y \Delta t}{(\Delta y)^2}\left(C_{i,j+1}^k - 2C_{i,j}^k + C_{i,j-1}^k\right) - \frac{v_x}{\Delta x}\left(C_{i+1,j}^k - C_{i,j}^k\right) - \frac{v_y}{\Delta y}\left(C_{i,j+1}^k - C_{i,j}^k\right) \tag{1.12}$$

For computational sophistication, the flow domain is discretized in N_x+1 and N_y+1 grid points, each of length Δx and Δy;

2.1 One-dimensional model

To illustrate the capabilities of the model to predict the effects of advection-dispersion of contaminant transport, here a finite difference model is applied to contaminant transport problem in a saturated unconfined aquifer of finite length with constant velocity and dispersion field. It demonstrate the effect of time, advection velocity and dispersion. Flow dynamics is explained in current graphs.

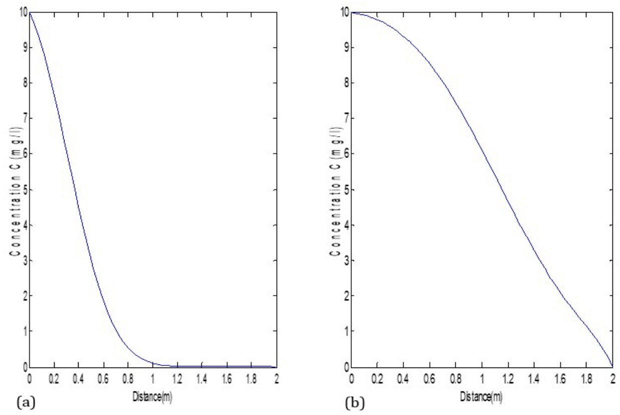

Fig. 2.1. Variation of contaminant with respect to distance for two different time duration when the parameters of Eq. (1.6) are given as $L = 2$ m, $D_x = 0.1$m²/day, $v_x = 0.5$ m/day, $Dt = 0.0005$ day, $Dx = 0.05$ m, (a) $T = 0.5$ day and (b) $T = 2$ day.

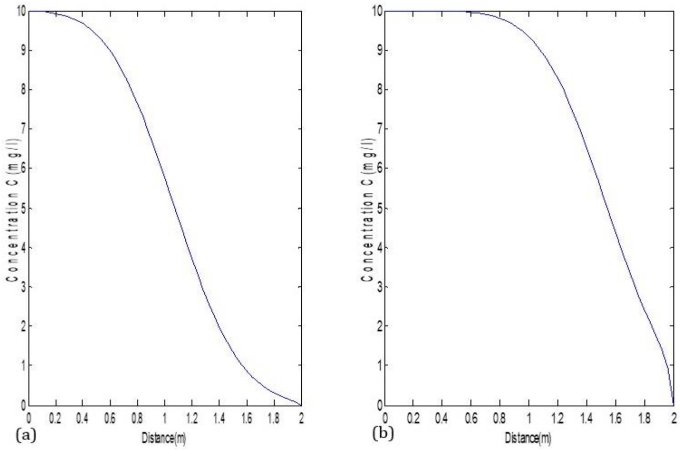

Fig. 2.2. Variation of contaminant with respect to distance for two different advection velocities, when the parameters of Eq. (1.6) are given as $L = 2$ m, $D_x = 0.1$m²/day,$T = 1$ day, $Dt = 0.0005$ day, $Dx = 0.05$ m, (a) $v_x = 1$ m/dayand (b) $v_x = 1.5$ m/day.

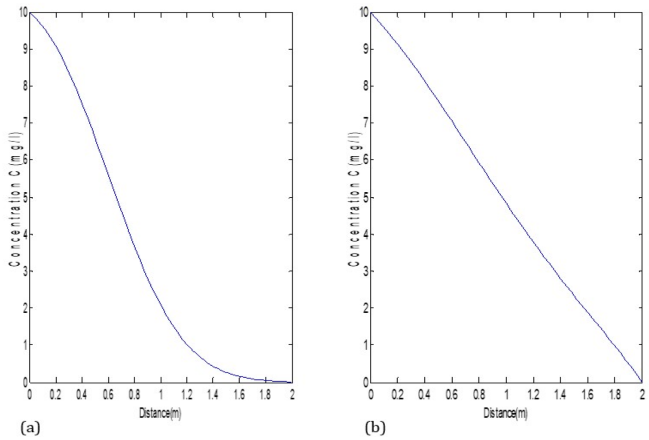

Fig. 2.3. Variation of contaminant with respect to the distance for two different dispersion coefficients, when the parameters of Eq. (1.6) are given as $L = 2$ m,$v_x = 0.5$ m/day,$T = 1$ day,$\Delta t = 0.0005$ day, $Dx = 0.05$ m, (a) $D_x = 0.12$m²/day (b) $D_x = 0.5$m²/day.

2.2 One-D model's results and discussion

(i) As the time of simulation increases from 0.5 day to 2-day, contaminant plume in direction of flow shifted from 1.2 m to 2 m. It is observed, as time progresses the contaminant plume shifted from one place to another place. As contaminant moves it disperses, fig. (2.1) shows that the concentration decreases when it moves far away from the source of contaminant. This is the main reason; concentration of contaminant is different at different locations in the aquifer at different time.

(ii) As advection velocity increases from 1 m/day to 1.5 m/day, concentration of contaminant dominated till 0.6 m, plume again shifted in direction of flow beyond 2 m. It shows as velocity increases, plume shifted from one position to other position at larger scale at the same instant of time. As explained in fig. (2.2), when contaminant plume moves it disperses, present graphs show that when advection velocity increases, contaminant plume disperses at faster rate and the contaminant spreads till farther location from the source.

(iii) As dispersion increases from 0.12 m²/day to 0.5 m²/day, concentration of contaminant changes with increase in dispersion at the same instant of time, it affects the spreading of contaminant plume at large scale in longitudinal directions as compare to advection velocity and time. As Fig. 2.3 (b) shows at steady state, plume is shifting from its position uniformly in forward and backward direction. If there is no dispersion, all of the contaminant will travel at same advection velocity. As dispersion increases, some contaminant travels faster and some slower. There are differences of velocity between particles, which causes spreading at larger scale. It shows, contaminant transport is affected more by dispersion as compare to advection.

3.1 Two-dimensional model

Now the idea of one-dimensional modeling is extended to model the two-dimensional advection-dispersion phenomenon in an unconfined saturated aquifer. A rectangular domain of length L along x-axis and width of B along y-axis is taken for the present study. The origin of the flow domain is taken at O, which can be seen in Fig. 2.2. The dispersion and velocity field along x and y-directions are taken as D_x, D_y, v_x and v_y respectively. The present study deals with the different variations of velocity field and boundary conditions corresponding to flow diagram Fig. 2.2.

Case 1: Constant velocity field along *x* and *y*-direction with different Dirichlet conditions along four faces.

In this study, a constant velocity field is taken along both the directions, whereas the boundaries along $x = 0,\ x = L,\ y = 0$, and $y = B$ are taken as $C_2,\ C_4,\ C_3$ and C_1 respectively. The mathematical expressions for the same are given by Eqs. (2.2), (2.3), (2.4) and (2.5) respectively. An explicit finite difference methodology is used to obtain the solution of Eq. (1.2) subjected to these boundary conditions. The initial condition of the flow domain is taken as zero. Thus

$$C(x, y, 0) = 0 \qquad (2.1)$$

Concentration of contaminants at the entire boundary is given by

$C(x,0,t)=C_3$ (2.2)

$C(x,B,t)=C_1$ (2.3)

$C(0,y,t)=C_2$ (2.4)

$C(L,y,t)=C_4$ (2.5)

Fig. 2.4. illustrates the variation of contaminants concentration with respect to the distance for two different time duration when the parameters of Eq. (1.12) are given as

$L=1\,\text{m},\ B=1\,\text{m},\ D_x=2\,\text{m}^2/\text{day},\ D_y=2\,\text{m}^2/\text{day},$
$v_x=1\,\text{m/day},\ v_y=1\,\text{m/day},\ \Delta x=0.05\,\text{m},$
$\Delta y=0.05\,\text{m},\ \Delta t=0.5\,\text{sec},$ (a) $T=250\,\text{sec},$ (b) $T=4000\,\text{sec}.$

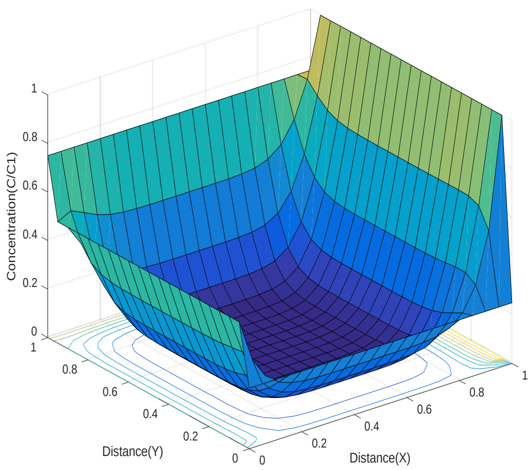

Fig.2.4. (a) variation of contaminants concentration at T=250 sec.

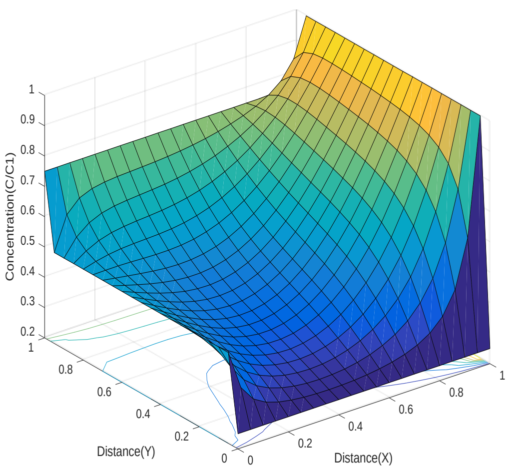

Fig.2.4. (b) variation of contaminants concentration at T=4000 sec.

Case 2: Different velocity field along *x* and *y*-direction with different linearly varying Dirichlet conditions along four faces.

This study deals with more general boundary conditions imposition as compared to case 1. The concentrations at the extreme edges of the flow domain are taken as C_1, C_2, C_3 and C_4. However, the distributions of concentrations along any edge line are taken as linear.

For the boundary $y=0$, the variation of concentration is from C_2 to C_3 varying linearly, which can be observed from Eq. (2.7) and for boundary $y=B$ the variation of concentration C_1 to C_4 linearly, observed from Eq. (2.8). Similarly, for boundary $x=0$, the variation of concentration is from C_2 to C_1 varying linearly which is given by Eq. (2.9) and for boundary $x=L$, the variation of concentration is from C_3 to C_4 which is expressed by Eq. (2.10). The initial condition for the above-mention problem is taken as

$C(x,y,0)=0$ (2.6)

Concentration of contaminants at all the boundaries are given by

$$C(x,0,t)=C_2\left(\frac{L-x}{L}\right)+C_3\left(\frac{x}{L}\right) \quad (2.7)$$

$$C(x,B,t)=C_1\left(\frac{L-x}{L}\right)+C_4\left(\frac{x}{L}\right) \quad (2.8)$$

$$C(0,y,t)=C_2\left(\frac{B-y}{B}\right)+C_1\left(\frac{y}{B}\right) \quad (2.9)$$

$$C(L,y,t)=C_3\left(\frac{B-y}{B}\right)+C_4\left(\frac{y}{B}\right) \quad (2.10)$$

Fig. 2.5. illustrates the variation of contaminants concentration with respect to the distance for two different time duration when the parameters of Eq. (1.12) are given as

$L=1\,\text{m},\ B=1\,\text{m},\ D_x=2.7\,\text{m}^2/\text{day},\ D_y=2.2\,\text{m}^2/\text{day},$
$v_x=2\,\text{m/day},\ v_y=6\,\text{m/day},$
$\Delta x=0.05\,\text{m},\ \Delta y=0.05\,\text{m},\ \Delta t=0.5\,\text{sec},$ (a) $T=250\,\text{sec},$ (b) $T=500\,\text{sec},$ (c) $T=5000\,\text{sec}$

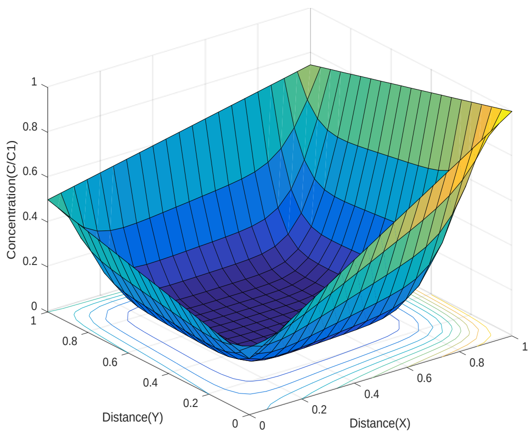

Fig.2.5. (a) variation of contaminants concentration at T=250 sec

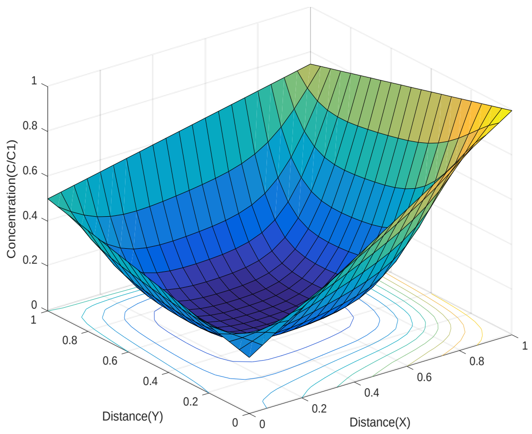

Fig.2.5. (b) variation of contaminants concentration at T=500 sec.

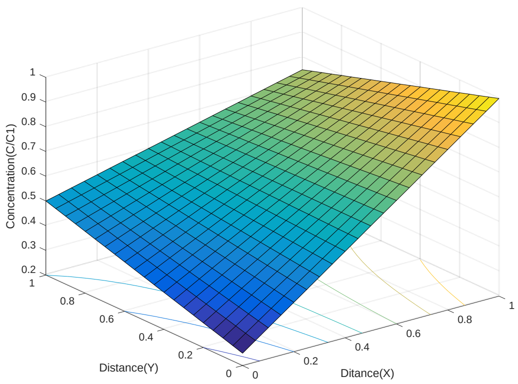

Fig.2.5. (c) variation of contaminants concentration at T=5000 sec.

Case 3: Varying velocity field along *x* and *y*-direction with different Dirichlet conditions along four faces.

The concentrations at the extreme edges are distributed uniformly in the flow domain. Are taken as C_1, C_2, C_3 and C_4 respectively. For the boundary $y=0$, concentration is C_3, which can be observed from Eq. (2.12). Similarly for the boundary $y=B$, concentration is C_1, observed by Eq. (2.13). For boundary $x=0$, concentration is C_2, which can be observed by Eq. (2.14). Similarly for boundary $x=L$, concentration is C_4, observed by Eq. (2.15).

The initial condition for the above-mention problem is taken as

$$C(x,y,0)=0 \qquad (2.11)$$

Concentration of contaminants at all the boundary is given by following equations –

$$C(x,0,t)=C_3 \qquad (2.12)$$

$$C(x,B,t)=C_1 \qquad (2.13)$$

$$C(0,y,t)=C_2 \qquad (2.14)$$

$$C(L,y,t)=C_4 \qquad (2.15)$$

Fig. 2.6. illustrates the variation of contaminants concentration with respect to the distance for two different time duration when the parameters of Eq. (1.12) are given as

$\boldsymbol{L} = \mathbf{1.5}$ **m**, $\boldsymbol{B} = \mathbf{1.5}$ **m**, $D_x = 2\,\mathrm{m}^2/\mathrm{day}$,
$\boldsymbol{D_y} = \mathbf{2}\ \mathbf{m^2/day}$,
$v_x = (1+x)(1+y)$,
$\boldsymbol{v_y} = (\mathbf{1}+\boldsymbol{x})(\mathbf{1}+\boldsymbol{y})$, $\boldsymbol{\Delta x} = \mathbf{0.05}$ **m**, $\boldsymbol{\Delta y} = \mathbf{0.05}$ **m**, $\boldsymbol{\Delta t} = \mathbf{0.5}$ **sec**,
(a) $\boldsymbol{T} = \mathbf{250}$ **sec**, (b) $\boldsymbol{T} = \mathbf{4000}$ **sec**.

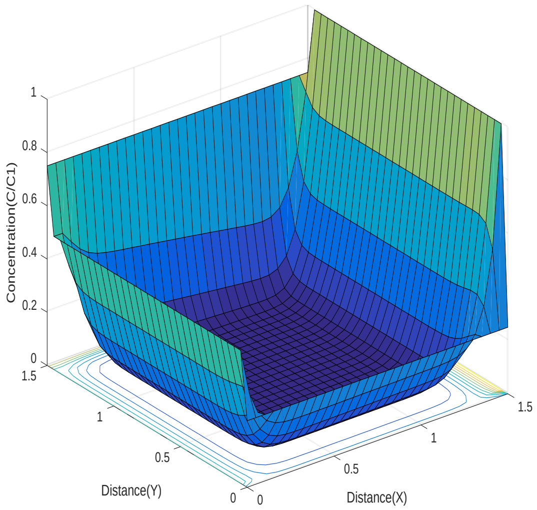

Fig. 2.6. (a) variation of contaminants concentration at T=240 sec.

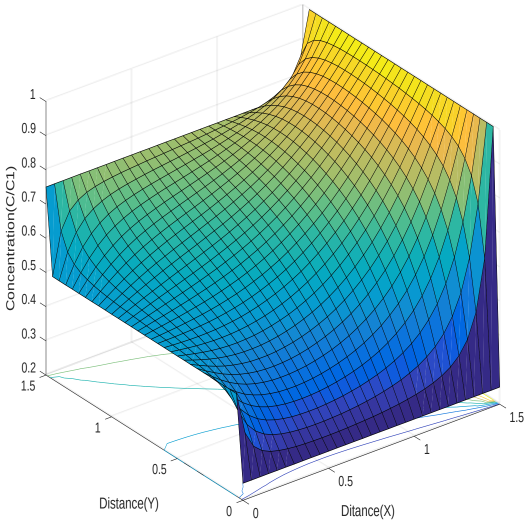

Fig. 2.6. (b) variation of contaminants concentration at T=4000 sec.

3.2 Two-dimensional model results

(i) Fig. 2.4. (a) clearly shows that maximum contamination occurs first somewhere close to corner of contamination. Advection velocity is same in both directions, so contaminant plume starts shifting from one place to other place at same rate. As distance increasing, contaminant concentration decreasing uniformly in both direction from all its initial values. It is observed that when the values of x and y approaches beyond 2 m then concentration of contaminant is minimum in this region.

(ii) Figure 2.4. (b) shows the steady state of contaminants as the time passes beyond 4000 sec, contaminant will not spread more than the present concentration. Here it is observed that for two-dimensional domain also as time progresses dispersion of contaminant increases to full extent.

(iii) Fig. 2.5. (a) clearly shows concentration of contaminants is varying linearly at all boundaries. Here advection velocity is not same in both the direction, so contaminant plume shifts from one place to other at different rate in both directions. As the distance is increasing, the contaminant concentration decreasing from all its initial values. Here also, it is observed that when the values of x and y approaches beyond 0.2 m then concentration of contaminant is minimum in this region.

(iv) Fig. 2.5. (b) shows when the contaminant concentration increased beyond 0.4 m distance in x and y direction, region of minimum concentration starts beyond this distance. This region is smaller as compare to Fig. 2.5. (a) due to progress in time which causes more dispersion. As previous case discusses when time progresses dispersion increases due to the movement of contaminants by advection velocity.

(v) Fig. 2.5. (c) shows the steady state condition where the contaminants disperse to its maximum extent for the given parameters. Beyond this time, the concentration of the contaminates will attain its peak value throughout domain; the system has reached to its saturation which can be observed from Fig.2.5. (c).

(vi) For this case also Fig. 2.6. (a) clearly shows that maximum contamination occurs first somewhere close to corner of contamination. Here advection velocity is changing according to the position of x and y in both directions, so contaminant plume is shifting from one place to other place at different rate at different position in the region. It is observed that when the values of x and y approaches beyond 0.1 m then concentration of contaminant is minimum in this region. Here this region is larger than previous all cases. Fig. 2.6. (b) shows the steady state condition at 4000 sec for given parameters.

4. CONCLUSIONS

The present study involves the modeling of one and two-dimensional contaminant transport phenomenon in an unconfined aquifer by solving advection-dispersion equation for a given sets of initial and boundary conditions using finite difference formulation. The study covers the results of one-dimensional modeling in the first step, in which three sub-cases corresponding to different values of dispersion, advection velocity is considered for the study. For further step this study is extended to the two-dimensional domain, where the movement of contaminants is observed for three different cases. The study through insight to the distribution and transport phenomenon of the contaminants in a rectangular domain subjected to different combination of boundary conditions. With the help of these models, we can predict the contaminant concentration at different location in a flow domain at different times. This study has also shown the improvements in the simulation of the transport of contaminants arising from using a two-dimensional advection-dispersion equation. Contaminant transport is examined in unconfined aquifer according to specific boundary conditions along with the assumption of constant dispersion coefficients throughout the domain.

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