SIMULATION AND MODELING TECHNIQUE DEVELOPMENT FOR UNSTEADY CONTAMINANTS TRANSPORT PROBLEMS IN SATURATED SUBSURFACE HETEROGENEOUS MEDIUMS [+]

تطوير تقنية التمثيل والنمذجة الرياضية لمشاكل انتقال الملوثات المتغيرة في الاوساط التحت سطحية الغير متجانسة المشبعة

Najah M. L. Al-Maimuri [*]

المستخلص:

لقد طور برنامج حاسوبي والذي بواسطته يمكن تمثيل انتقال الملوثات بخاصية الانتقال والانتشار في الاوساط الغير متجانسة ببعد واحد واثنين وثلاثي الابعاد متغير الزمن في المياه التحت سطحية. ان تقنيات البرمجة تضمنت تغير الزمن وملوثات نقطية وخطية ومساحية بدون التطرق الى الملوثات النبضية.

ان شرح تقنية النمذجة الرقمية تضمنت الخلفية الرياضية النظرية وقائمة البرنامج وطريقة النمذجة. ان نظرية الفروقات المحدده قد استعملت لتمثيل ظاهرة الانتقال والانتشار. ان طريقة الاتجاهات الضمنية المتناوبة المعدلة قد استعملت لحل مجموعة معادلات الفروقات المحددة. ان البرنامج المدرج قد كتب في لغة فورتران ٤ ويعمل بكل انواع الوحدات. بعد تشغيل النموذج وجد ان الملوث بتركيز ١٠٠٠ملغم\لتر في الحد الشرقي يصل الى النهر بعد ٩٠٥،٦ يوم من بداية تشغيل النموذج.

Abstract:

A general computer program listing is developed that can mathematically simulate one, two, and three dimensional non-steady advection-dispersion contaminant transport in a heterogeneous subsurface media. Programming techniques, involving time varying, point, line and/or area sources of contamination but not a pulsing contamination on the media.

The discussion of the modeling digital techniques includes the necessary mathematical background documented program listing, and job setup procedure. A finite difference approach is used to derive and formulate the equations of advection dispersion phenomena. A modified alternating direction digital implicit method is used to solve the set of resulting finite difference equations. The program included is written in *FORTRAN IV* and operates with any set of units. After the model has been run, it is found that the pollutant of concentration 1000mg/liter at the western polluted boundary reaches the river with concentration of 96mg/liter after a period of 905.6days since the model started.

[+] **Received on 6/4/2011 , Accepted on**

[*] **Asist .Lecturer / Babylon Tech. Institute**

Introduction:

The main object of this study is to present a generalized computer program that will simulate one, two, and three dimensional unsteady state advection dispersion problems in heterogeneous groundwater media. The program covers time varying and contaminated point, line and/or area sources. A finite difference approach is adopted .

Bear [1] presented the tracer distribution caused by dispersion in one and two-dimensional flow. It has been experimentally verified that the testing of the transition zone depends upon the path of the mean point and is independent of the flow velocity. Rumer [2] obtained longitudinal dispersion coefficients using a one-dimensional dispersion model in which the average velocity is constant throughout the length of the flow field. Harleman and Rumer [3] measured the coefficients of longitudinal and lateral dispersion for steady uniform flow through an isotropic porous medium. List and Brooks [4] studied the relationship between the lateral dispersion and the Peclet number. It was found that the lateral dispersion is dependent on the viscosity when the flow is linear-laminar (low Reynolds number). Narasimhan and Witherspoon [5] because of the difficulty in obtaining analytical solutions to groundwater flow and mass transport, many investigations have been done using numerical methods. During mid-1960's, the finite element method has developed into a powerful numerical tool for analyzing a variety of groundwater flow and pollution problems. Smith et al [6] presented finite element methods for the solution of diffusion-convection problems. Galerkin elements are used with equal weight for diffusion and convection as a physical modeling process. Frind [7] undertook the problem of contaminant transport by using a new simulation technique based on Galerkin finite elements, but formulated in terms of principal directions of transport. It is proved that the new technique is more accurate and efficient than conventional finite element technique. Peter and Jozef [8] described a new method to determine semi-analytical solutions of one-dimensional contaminant transport problem with non-linear sorption. It is based on splitting approach where the convection transport is solved exactly. Peter [9] discussed the application of the finite element method to the numerical solution of scalar two dimensional steady convection-diffusion equations with the emphasis on upwinding techniques satisfying the discrete maximum principle.

Mirbagheri [10] A mathematical and computer model for the transport and transformation of solute contaminants through a soil column from the surface to the groundwater is presented. The model simulates selenium species such as selenate, selenite, and selenomethionine as well as pesticides and nitrogen. This model is based on the mass balance equation including convective transport, dispersive transport, surface adsorption, oxidation and reduction, volatilization, chemical and biological transformation. The governing equations are solved numerically by the method of implicit finite difference. The simulation results are in good agreement with measured values. The major finding in the present study indicates that as the time of simulation increases, the concentration of different selenium species approaches the measured values.

The current analysis is similar to the numerical approaches of Prickett and Lonngquist [11] and Pinder and Bredehoeft [12] which are governed by a finite difference form of the partial differential equation of groundwater flow.

Study Objectives:

The study is aimed to add the following contributions to ecosystem

1- Developing and conceptualizing a mathematical simulation technology of subsurface contaminant transport in saturated mediums.

2- Analyzing a field problem by using the current new technology.

Mathematical Solution:

The beginning of the solution of the 3D advection dispersion equation of the form:

$$[D_x\frac{\partial 2C}{\partial x^2}+D_y\frac{\partial 2C}{\partial y^2}+D_z\frac{\partial 2C}{\partial z^2}]-\left[v_x\frac{\partial C}{\partial x}+v_y\frac{\partial C}{\partial y}+v_z\frac{\partial C}{\partial z}\right]=\frac{\partial C}{\partial t}+Q_c \quad \text{.....(1)}$$

Where: D is the dispersion coefficient, □ is the ground water velocity, and C is the volumetric concentration in the media

To compromise Eq. (1) to be fitted to the water table condition it may be reduced to two-dimensional problem as:

$$[D_x\frac{\partial 2C}{\partial x^2}+D_y\frac{\partial 2C}{\partial y^2}]-\left[v_x\frac{\partial C}{\partial x}+v_y\frac{\partial C}{\partial y}\right]=\frac{\partial C}{\partial t}+Q_c \quad \text{.....(2)}$$

Where $+Q_c$ is termed for sink and/or source volumetric concentration discharge

To solve Eq. (2) numerically by using the finite difference approximation, the Taylor series expansion is technically fit to proceed. Briefly, the first and second derivatives in x-axis according to Taylor are as follows: Erwin Kreyszig [13]

$$\frac{\partial C}{\partial x_{i,j}}=\frac{C_{i+1,j}-C_{i,j}}{\Delta x} \quad \text{.....(3)}$$

$$\frac{\partial 2C}{\partial x^2{}_{i,j}}=\frac{C_{i+1,j}-C_{i,j}+C_{i-1,j}}{\Delta x^2} \quad \text{.....(4)}$$

Similarly, the first and second derivatives in ordinate axis are as follows:

$$\frac{\partial C}{\partial y_{i,j}}=\frac{C_{i,j+1}-C_{i,j}}{\Delta y} \quad \text{.....(5)}$$

$$\frac{\partial 2C}{\partial y^2{}_{i,j}}=\frac{C_{i,j+1}-C_{i,j}+C_{i,j-1}}{\Delta y^2} \quad \text{.....(6)}$$

$$\frac{\partial C}{\partial t_{i,j}}=\frac{C_{i,j}+Co_{i,j}}{\Delta t} \quad \text{..... (7)}$$

Where $C_{i,j}$ is the volumetric concentration at any time, $Co_{i,j}$ is the initial volumetric concentration, Δt is the time step within the time domain and the subscript i,j is adapted to help in understanding of direction in the complex analytical terminology.

By substitution of the expansions of Eqs. (3,4,5,6,7) into Eq. (2).

$$D_{i,j,1}\frac{C_{i+1,j}-2C_{i,j}+C_{i-1,j}}{\Delta x^2}-v_{i,j,1}\frac{C_{i+1,j}-C_{i,j}}{\Delta x}+D_{i,j,2}\frac{C_{i,j+1}-2C_{i,j}+C_{i,j-1}}{\Delta y^2}-v_{i,j,2}\frac{C_{i,j+1}-C_{i,j}}{\Delta y}=\frac{C_{i,j}-Co_{i,j}}{\Delta t}+QC_{i,j} \quad \text{..... (8)}$$

For expansion of the solution through the modeling process, a non-equal mesh dimensions to be used. This leads to $\Delta x \neq \Delta y$, if we assume that if the dispersing is nonhomogeneous ($D_{i,j,1} \neq D_{i,j,2}$) and by multiplication and rearranging Eq. (8) becomes:

$$\frac{D_{i,j,1}}{\Delta x_{i,j}^2}C_{i-1,j}+\left[\frac{D_{i,j,1}}{\Delta x_{i,j}^2}-\frac{v_{i,j,1}}{\Delta x_{i,j}}\right]C_{i+1,j}+\left[\frac{2D_{i,j,1}}{\Delta x_{i,j}^2}+\frac{v_{i,j,1}}{\Delta x_{i,j}}+\frac{2D_{i,j,2}}{\Delta y_{i,j}^2}+\frac{v_{i,j,2}}{\Delta y_{i,j}}-\frac{1}{\Delta t}\right]C_{i,j}+\frac{D_{i,j,2}}{\Delta y_{i,j}^2}C_{i,j-1}+\left[\frac{D_{i,j,2}}{\Delta y_{i,j}^2}-\frac{v_{i,j,2}}{\Delta y_{i,j}}\right]C_{i,j+1}=-\frac{Co_{i,j}}{\Delta t}+QC_{i,j}$$

.....(9)

Iterative Alternating Direction Implicit Method

Briefly, the iterative alternating direction implicit method involves first for a given time increment, reducing a large set of simultaneous equation down to a number of small set. This is done by Guass elimination solution to the node equation. According to Peaceman and Rachford [14], the set of column equations is then implicit in the direction along the column and explicit in the direction of orthogonal to the column alignment, then the solution of column set equation is a straight forward process.

After all column equations have been processed column by column, the solution of node equations set is carried out again by gauss elimination of an individual row while all terms related to adjacent rows are held constant. Eventually, after all node equations have been solved row by row, the above process is repeated for a sufficient number of times until a convergent is obtained. The above solution process should be repeated for each time increment. Peaceman and Rachford [14] indicated that this technique is unconditionally stable regardless of the time increment size. Accordingly Eq. (9) should be modified and arranged to facilitate the columns and rows solving technique.

For solving Eq. (9) by columns, it may be rearranged as:

$$\frac{D_{i,j,2}}{\Delta y_{i,j}^2} C_{i,j-1} + \left[\frac{2D_{i,j,1}}{\Delta x_{i,j}^2} + \frac{v_{i,j,1}}{\Delta x_{i,j}} + \frac{2D_{i,j,2}}{\Delta y_{i,j}^2} + \frac{v_{i,j,2}}{\Delta y_{i,j}} - \frac{1}{\Delta t}\right] C_{i,j} + \left[\frac{D_{i,j,2}}{\Delta y_{i,j}^2} - \frac{v_{i,j,2}}{\Delta y_{i,j}}\right] C_{i,j+1}$$
$$= -\frac{D_{i,j,1}}{\Delta x_{i,j}^2} C_{i-1,j} - \left[\frac{D_{i,j,1}}{\Delta x_{i,j}^2} - \frac{v_{i,j,1}}{\Delta x_{i,j}}\right] C_{i+1,j} - \frac{Co_{i,j}}{\Delta t} + Qc_{i,j} \quad \ldots\ldots\ldots (10)$$

Eq. (10) of the form

$$AA_j C_{i,j-1} + BB_j C_{i,j} + CC_j C_{i,j+1} = DD_j \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

Where the coefficient terms are:

$$AA_j = \frac{D_{i,j,2}}{\Delta y_{i,j}^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (11a)$$

$$BB_j = \left[\frac{2D_{i,j,1}}{\Delta x_{i,j}^2} + \frac{v_{i,j,1}}{\Delta x_{i,j}} + \frac{2D_{i,j,2}}{\Delta y_{i,j}^2} + \frac{v_{i,j,2}}{\Delta y_{i,j}} - \frac{1}{\Delta t}\right] \quad \ldots\ldots\ldots\ldots\ldots (11b)$$

$$CC_j = \left[\frac{D_{i,j,2}}{\Delta y_{i,j}^2} - \frac{v_{i,j,2}}{\Delta y_{i,j}}\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (11c)$$

$$DD_j = -\frac{D_{i,j,1}}{\Delta x_{i,j}^2} C_{i-1,j} - \left[\frac{D_{i,j,1}}{\Delta x_{i,j}^2} - \frac{v_{i,j,1}}{\Delta x_{i,j}}\right] C_{i+1,j} - \frac{Co_{i,j}}{\Delta t} + Qc_{i,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (11d)$$

For solving Eq. (10) in term of row formulation, it may be rearranged to be as:

$$\frac{D_{i,j,1}}{\Delta x_{i,j}^2} C_{i-1,j} + \left[\frac{2D_{i,j,1}}{\Delta x_{i,j}^2} + \frac{v_{i,j,1}}{\Delta x_{i,j}} + \frac{2D_{i,j,2}}{\Delta y_{i,j}^2} + \frac{v_{i,j,2}}{\Delta y_{i,j}} - \frac{1}{\Delta t}\right] C_{i,j} + \left[\frac{D_{i,j,1}}{\Delta x_{i,j}^2} - \frac{v_{i,h,1}}{\Delta x_{i,j}}\right] C_{i+1,j}$$
$$= -\frac{D_{i,j,2}}{\Delta y_{i,j}^2} C_{i,j-1} - \left[\frac{D_{i,j,2}}{\Delta y_{i,j}^2} - \frac{v_{i,j,2}}{\Delta y_{i,j}}\right] C_{i,j+1} - \frac{Co_{i,j}}{\Delta t} + Qc_{i,j} \quad \ldots\ldots (12)$$

Eq. (12) of the form

$$AA_i C_{i-1,j} + BB_i C_{i,j} + CC_i C_{i+1,j} = DD_i \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (13)$$

Where the coefficient terms are:

$$AA_i = \frac{D_{i,j,1}}{\Delta x_{i,j}^2} \quad \ldots\ldots (13a)$$

$$BB_i = \left[\frac{2D_{i,j,1}}{\Delta x_{i,j}^2} + \frac{v_{i,j,1}}{\Delta x_{i,j}} + \frac{2D_{i,j,2}}{\Delta y_{i,j}^2} + \frac{v_{i,j,2}}{\Delta y_{i,j}} - \frac{1}{\Delta t}\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots (13b)$$

$$CC_i = \left[\frac{D_{i,j,1}}{\Delta x_{i,j}^2} - \frac{v_{i,j,1}}{\Delta x_{i,j}}\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (13c)$$

$$DD_i = -\frac{D_{i,j,2}}{\Delta y_{i,j}^2} C_{i,j-1} - \left[\frac{D_{i,j,2}}{\Delta y_{i,j}^2} - \frac{v_{i,j,2}}{\Delta y_{i,j}}\right] C_{i,j+1} - \frac{Co_{i,j}}{\Delta t} + Qc_{i,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (13d)$$

There are three unknown concentrations of each equation whether for columns Eq. (11) or for row Eq. (13). [In standard matrix notation a set of equations presented by Eq. (11) or Eq. (13) forms what is mathematically termed as tri-diagonal matrix]. The solution of a set of columns or rows concentration is carried out by Guass-Elimination interpolating what Peaceman and Rachford [14] term A and B arrays applied to tri-diagonal matrices.

Calculation Setup of Concentrations with A and B Arrays

An example could be used to show how concentrations are calculated with the use of A and B arrays. Although the current method applied to any number of nodes in a row or column, a four nodes row-column as in Fig. (1) is considered.

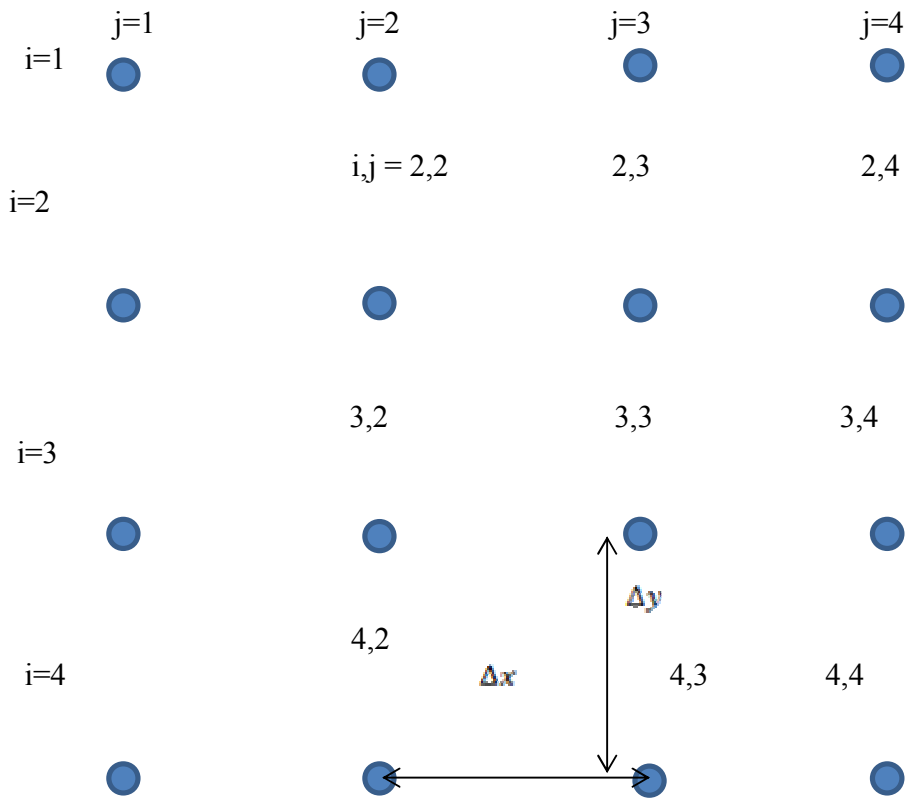

Fig. (1) Four Nodes row-Column Mesh Design and Direction of Reading Initialization

The concentrations at the nodes 1,2, 3, and 4 along ith row can be calculated by first writing the row equations [of the form Eq. (14)] for each node going in order of increasing column number (j). Secondly, the resulting equations are arranged in such a manner that the concentration at each node of interest $C_{i,j}$ is a function of known parameter of the last node $C_{i-1,j}$, if this is done all other concentrations can sequentially be calculated in order of increasing column number.

At the first jth row node, i=1 and the centration is of the form

$$AA_1C_{0,j} + BB_1C_{1,j} + CC_1C_{2,j} = DD_1 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (14)$$

Since no node with coordinates (0.j), therefore AA_1 is set to be zero and Eq. (14) is reduced to:

$$BB_1C_{1,j} + CC_1C_{2,j} = DD_1 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (14a)$$

Eq. (15a) may be rearranged into:

$$C_{1,j} = \frac{DD_1}{BB_1} - \frac{CC_1}{BB_1}C_{2,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (14b)$$

If $A_1 = \frac{DD_1}{BB_1}$, and $B_1 = \frac{CC_1}{BB_1}$, then Eq. (14b) becomes

$$C_{1,j} = A_1 - B_1C_{2,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (14c)$$

Now the concentration at the node of interest $C_{1,j}$ is a function of known parameters A_1 and B_1 and the concentration at only the node $C_{i+1,j}$ or $C_{2,j}$. Proceeding to the next jth row node of Fig. (1) where i=2, the concentration equation is

$$AA_2C_{1,j} + BB_2C_{2,j} + CC_2C_{3,j} = DD_2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (15)$$

The solution for $BB_2C_{2,j}$ gives

$$BB_2C_{2,j} = DD_2 - CC_2C_{3,j} - AA_2C_{1,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (15a)$$

Substitute Eq. (14c) into Eq. (15a) to obtain

$$BB_2C_{2,j} = DD_2 - CC_2C_{3,j} - AA_2(A_1 - B_1C_{2,j}) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (15b)$$

Carrying out multiplication, rearranging and solving for $C_{2,j}$

$$C_{2,j} = \frac{DD_2 - AA_2A_1}{BB_2 - AA_2B_1} - \frac{CC_2}{BB_2 - AA_2B_1}C_{3,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (15c)$$

The known parameters of Eq. (15c) are defined as:

$$A_2 = \frac{DD_2 - AA_2A_1}{BB_2 - AA_2B_1}$$

$$B_2 = \frac{CC_2}{BB_2 - AA_2B_1}$$

Substitution of A_2 and B_2 into Eq. (15c) to obtain

$$C_{2,j} = A_2 - B_2C_{3,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (15d)$$

Proceeding to the next jth row where i=3, the concentration equation can be written as:

$$AA_3C_{2,j} + BB_3C_{3,j} + CC_3C_{4,j} = DD_3 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (16)$$

Similarly, the solution for $BB_3C_{3,j}$ gives

$$C_{3,j} = A_3 - B_3C_{4,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (16a)$$

Where:

$$A_2 = \frac{DD_2 - AA_2 A_2}{BB_2 - AA_2 B_2}$$

$$B_2 = \frac{CC_2}{BB_2 - AA_2 B_2}$$

Now and finally, the equation is written for the last jth row node i=4, then it becomes

$$AA_4 C_{3,j} + BB_4 C_{4,j} + CC_4 C_{5,j} = DD_4 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (17)$$

Since $C_{5,j}$ is not exist, then CC_4 is set to be zero which leads Eq. (17) to be zero

$$AA_4 C_{3,j} + BB_4 C_{4,j} = DD_4 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (17a)$$

By using the same analysis to Eq. (17a) to obtain

$$C_{4,j} = A_4 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (17b)$$

Where: $A_4 = \frac{DD_4 - AA_4 A_3}{BB_4 - AA_4 B_3}$

Since the concentration $C_{4,j}$ is now known, then a back substitution allows the other values of $C_{3,j}$ $C_{2,j}$ and $C_{1,j}$, Similarly all other concentrations in the jth row can be determined.

From the above manipulation, a general form for A and B terms can be written as:

$$A_N = \frac{DD_N - AA_N A_{N-1}}{BB_N - AA_N B_{N-1}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (18)$$

$$B_N = \frac{CC_N}{BB_N - AA_{N1} B_{N-1}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (19)$$

Where $N = i$ is specified for row calculation and by $N = j$ is specified for column calculation. In addition AA_N and CC_N are set equal to zero for the first and last row and column respectively.

Sets of equations of the form given by equations (18 and 19) for the nodes along a row or column are what Peacman and Rachford [14] term the A and B arrays are extremely computer storage and execution time.

A general form of equations (14c, 15d, 16a, and 17b) for row calculation can be written as

$$C_{i,j} = A_i - B_i C_{i+1,j} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (21)$$

Similarly, the general form of concentration equation for column calculation as

$$C_{i,j} = A_j - B_j C_{1,j+1} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (22)$$

In summary, the process of calculating the concentrations along columns or rows in the digital model includes first computing the A and B values, (Eqs. 19, 20) for nodes of columns or rows in order of increasing j or I respectively. After the last node concentration has been found, Eqs. (21, 22) are used to solve for all others concentration in the column or row in order of decreasing j or i respectively. After completing the calculation of the concentration in an individual column or row, the computer proceeds to the next column or row until all nodes in the digital model domain have been processed satisfactorily.

Basic Advection-Dispersion Simulation Program :

The technology of the program written by Prickett and Lonngquist [11] in water resources has been modified to fit the modeling of advection-dispersion problems because of its flexibility for modification and the ease for input and output data. Fig. (2) presents the listing of the program. Fig.(3) shows the flowchart sequential steps.

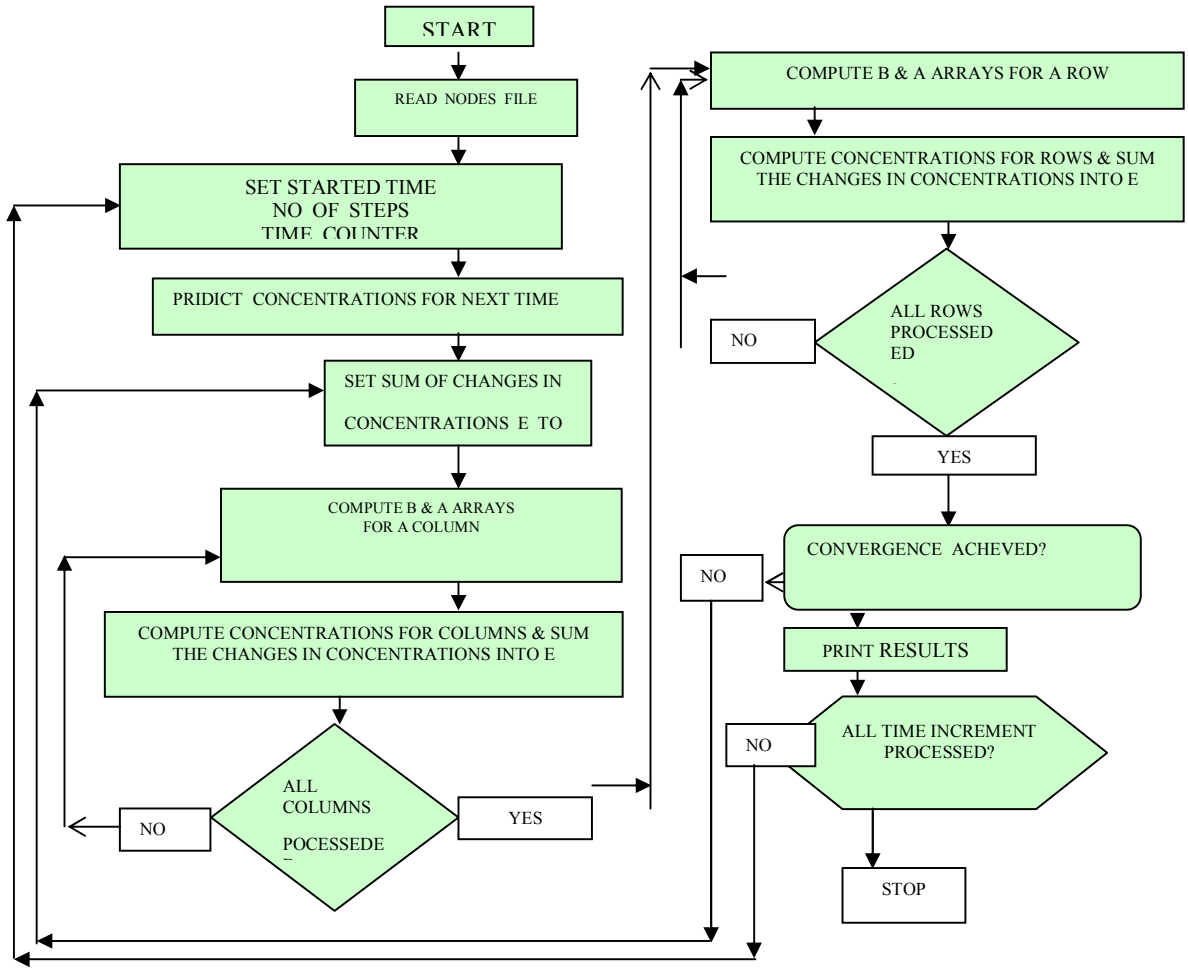

Fig.(3) Modified Simulation Flowchart of Advection Dispersion Contaminant Transport

Job Sequence and Data Input Files:

The first step in the sequence of modeling technology is beginning by superimposing a square finite deference mesh over the map interested domain as shown in Fig. (3). The Number of columns and rows are denoted by NC and NR respectively as outlined by Prickett and Lonnguist [11] . The boundary of the simulated aquifer is approximated by assigning zero diffusivity for all nodes outside the boundary. An initial contaminant concentration $Co_{i,j}$ is assigned for each node inside the model domain of Fig. (3). A dispersion coefficient is estimated and specified for each nodal point. A groundwater flow velocity in term of $v_{i,j,1}$ and $v_{i,j,2}$ is specified also for each node inside the model domain. Sink and source values of contamination concentration denoted by $Qc_{i,j}$ are specified for the nodes whenever they occur. A large value of dispersion coefficient is specified for all nodes located on the constant concentration source boundary. Two input data files are prepared for Δx & Δy dimensions in the case non-homogeneous mesh dimensions

```
                    PARAMETER (IMAX=110,JMAX=110)
                    IMPLICIT REAL*8 (A-H,O-Z)
                    DIMENSION C(IMAX),
                       C(IMAX,JMAX),CO(IMAX,JMAX),
                        Qc(IMAX,JMAX),D(IMAX),
SAMIR(IMAX,JMAX)
                    OPEN(1,FILE='AAA.DAT')
                    OPEN(2,FILE='BBB.RES')
                    OPEN(3,FILE='CCC.DAT')
                    OPEN(4,FILE='SAMIR.DAT')
                    OPEN(5,FILE='VVV.dat')
                    READ(1,*)NSTEPS,DELTA,ERROR,NC,NR,VEL,C
C,QQc,
                        DD
                    70 ,1.15E-5,.1,100,88, 0.05, 10,4.8,2,60, 50
C                   REMOVE NODES OUTSIDE THE MODELED
AREA
                    DO 520 J=1,NR
520                 READ(4,530)J,(SAMIR(I,J),I=1,NC)
530                 FORMAT(I3,2X,100F5.1)

CC                  KNCK = NUMBER OF GRID POINTS DIFFERENT
FROM
                        DEFAULT
C                   FILL ARRAYS WITH DEFAULT VALUES
                    DO 20 I=1,NC

                    DO 20 J=1,NR
                    V(I,J,1)=VEL
                    V(I,J,2)=VEL
                    D(I,J,1)=DD
                        D(I,J,2)=DD
                        VEL(I,J,1)=VEL
                        VEL(I,J,2)=VEL
                        C(I,J)=CC
                    Co(I,J)=CC
                    Qc(I,J)=QQc
20                  CONTINUE

C                   READ NODES FILES
                    KNCK =NC*NR
                        DO 22 K=1,KNCK

READ(3,*)I,J,V(I,J,1),V(I,J,2),D(I,J,1),D(I,J,2),Co(I,J), Qc(I,J)
22                  CONTINUE

C                   START OF SIMULATION
50                  TIME=0
                    DO 320 ISTEP=1,NSTEPS
                    TIME=TIME+DELTA
C                   PRIDICT CONCENTRATIONS FOR NEXT TIME
INCREAMENT
                    DO 70 I=1,NC
                    DO 70 J=1,NR
                    D1=C(I,J)-CO(I,J)
                    CO(I,J)=C(I,J)
                    F=1.0
                    IF(DL(I,J).EQ.0.0)GO TO 60
                    IF(ISTEP.GT.2)F=D1/DL(I,J)
                    IF(F.GT.5.)F=5.0
                    IF(F.LT.0.0)F=0.0
60                  DL(I,J)=D1
                    C(I,J)=C(I,J)+D1*F
                    IF(C(I,J).GT.Co(I,J))C(I,J)=Co(I,J)-.01
70                  CONTINUE
C
C                   REFINE ESTIMATE OF CONCENTRATIONS
                    ITER=0
80                  E=0.0
                    ITER=ITER+1
C                   ------------------------------------------------------
C                   column calculations
                    DO 190 JJ=1,NC
                    J=JJ
                    IF(MOD(ISTEP+ITER,2).EQ.1)J=NC-I+1
                    DO 170 I=1,NR
C
c                   calculate A and B arrays
                    AA=D(I,J,2)/(DY(I,J)**2)
                        BB=((2*D(I,J,1)/(DX(I,J)**2)+V(I,J,1)/DX(I,J)+
                        (2*D(I,J,2)/DY(I,J)**2)+        V(I,J,2)/DY(I,J)-
1/DELTA
                        CC=(D(I,J,2)/(DY(I,J)**2)-V(I,J,2)/(DY(I,J))
                        DD=0.0
                    IF(J-1)90,100,90

90                      DD=DD-(D(I,J,1)/DX(I,J)**2)*C(I-1,J)
100                     IF(I-NR)110,120,110
110                                 DD= DD-(D(I,J,1)/DX(I,J)**2-
V(I,J,1)/DX(I,J))*C(I+1,J)
120                     DD= DD- Co(I,J)/DELTA+Qc(I,J)
 60                 W=BB-AA*B(J-1)
                    B(J)=CC/W
170                 A(J)=(DD-AA*A(J-1))/W
c
c                   re-estimate concentrations
                    E=E+ABS(C(I,NR)-A(NR))
                    C(I,NR)=A(NR)
                    N=NR-1
180                 CA=A(N)-B(N)*C(I,N+1)
                    E=E+ABS(CA-C(I,N))
                    C(I,N)=CA
                    N=N-1
                    IF(N.GT.0)GOTO 180
190                 CONTINUE

C                       ------------------------------------------------------
c                   row calculations
                    DO 300 JJ=1,NR
                    J=JJ
                    IF(MOD(ISTEP+ITER,2).EQ.1)J=NR-J+1
                    DO 280 I=1,NC
                        Calculate A and B arrays
                        AA=D(I,J,1)/(DX(I,J)**2)
                    BB=((2*D(I,J,1)/(DX(I,J)**2)+V(I,J,1)/DX(I,J)+
                        (2*D(I,J,2)/DY(I,J)**2)+        V(I,J,2)/DY(I,J)-
1/DELTA
                        CC=(D(I,J,2)/(DX(I,J)**2)-V(I,J,2)/(DX(I,J))
                    IF(J-NC)210,220,210
210                 DD=                         DD-(D(I,J,2)/DY(I,J)**2-
V(I,J,2)/DY(I,J))*C(I,J+1)
220                 DD= DD- Co(I,J)/DELTA+Qc(I,J
270                 W=BB-AA*B(I-1)
                    B(I)=CC/W
280                 A(I)=(DD-AA*A(I-1))/W

c                   re-estimate concentrations
                    E=E+ABS(C(NC,J)-A(NC))
                    C(NC,J)=A(NC)
                    N=NC-1
290                 CA=A(N)-B(N)*C(N+1,J)
                    E=E+ABS(C(N,J)-CA)
                    C(N,J)=CA
                    N=N-1
                    IF(N.GT.0)GOTO 290

300                 CONTINUE
303                 IF(E.GT.ERROR)GOTO 80
                    DELTA=DELTA+DELTA2
311                 WRITE(2,310)TIME,E,ITER             ,ISTEP
310                 FORMAT(6X,'TIME=
',F12.1,2X,'DAYS'/6X,'ERROR=',F14.6,2X
                        1,'NUMBER OF ITERATIONS='I5,'ISTEP='I3)
                    DELTA=DELTA*1.2
                    IF(ISTEP.LT.NSTEPS)GOTO 315
315                 R=1
                    DO 320 J=1,NR
320                 WRITE(2,330)J,(C(I,J),I=1,NC)
330                 FORMAT(I2,2X,100F8.2)
                                    END
```

Fig. (2) Basic Advection-Dispersion Simulation Program under Water-Table Condition

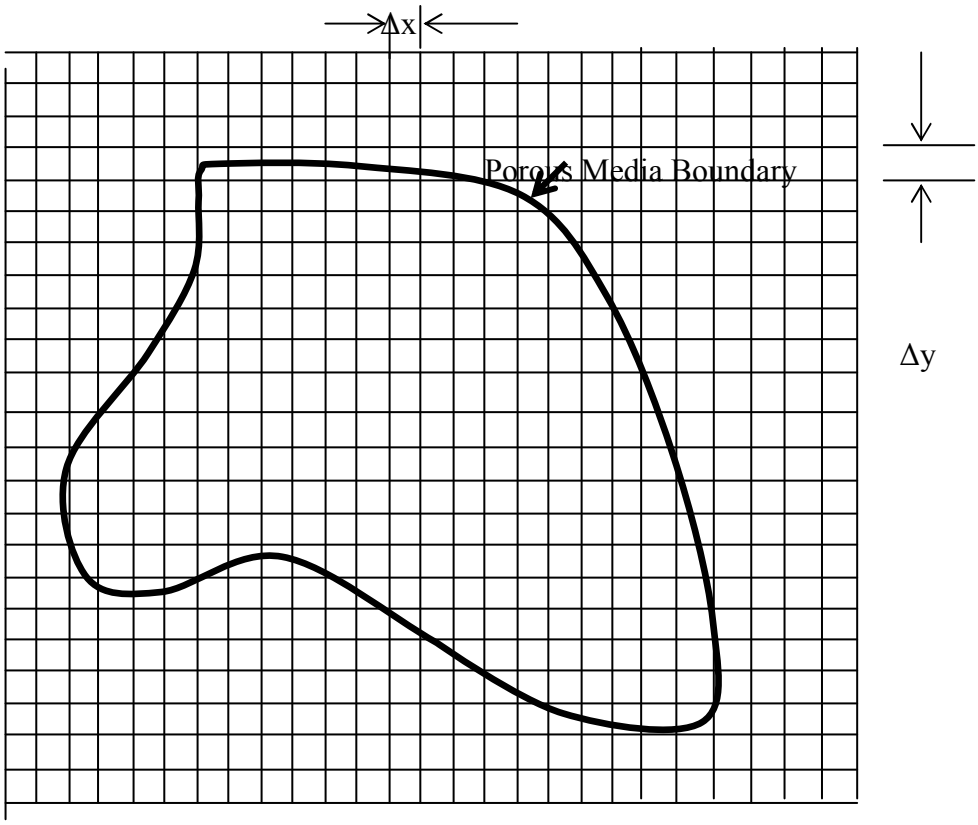

Fig. (3) Superimposing a Square Finite Deference Grids over a Model Domain

Infinite Groundwater Media Conditions:

I) Convergence Test and Errors

All computer programs of iterative nature should have an internal check on the error that is inherently occurred in solving finite difference equations. Many types of error checks are possible depending on the problem under study [11]. The error check in the simulation program assures that concentrations have converged to acceptable answer with a specified tolerance. The specified tolerance is predetermined or assumed and entered in the (aaa.dat) file. The term *error* represents the maximum allowable sum of the absolute values of the changes in concentration for all node points of the model during iteration. If the concentrations have no changed more than the error tolerance during the iterative process, the solution has converged to acceptable accuracy.

II) Program Iterative

High accuracy answers require more computer calculations which may be controlled by limiting the number of iterations. As the error term increased, the corresponding number of iterations per time delta decreased to meet the convergence of the solution.

III) *uniform Time Increment, Delta*

IV) Although small increments are needed for more accuracy where concentration changing rapidly (especially in the starting of contamination process) the small time increment becomes less important as the contamination process has proceeded.

V)Recharge Boundary Conditions

Point, line, and area boundaries are defined as boundaries at which there are no changes in water concentration. Those types of boundaries are most handled in the simulation process by setting the dispersion coefficient of the nodes along the position of the recharge boundaries to extremely large value.

Case Study & Model Validation:

To examine the model validity and the effect of the advection-dispersion parameters and field characteristics, an illustrative example is selected for this purpose. Fig.(4) represents the location map of the model domain. The current case study to be simulated by the model is to find out the value of the pollutant transport toward the river spatially and temporally within the model domain. It is supposed that the polluted boundary induces a certain amount of pollutant from the west toward the east to contaminate the river. Moreover, the study area shows that there is no flow of groundwater toward the north or south as a result of the natural existing boundary.

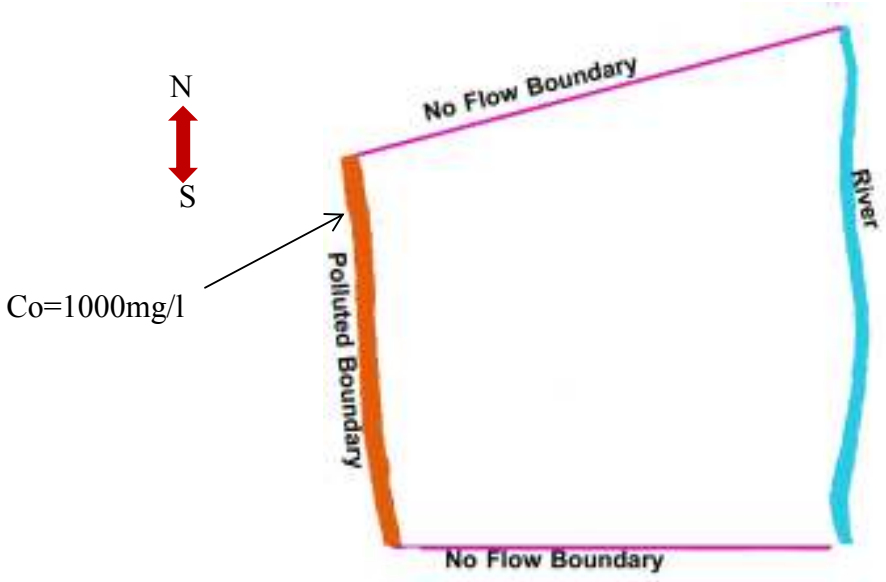

Fig.(4) Geographic map of the Model Area Under study

Discretization of the Domain

A square paper is superimposed over the geographic map to discretize the domain of the considered area into a suitable number of meshes. It is found that the number of columns $NC = 36$ and the number of rows NR$= 35$. The current descretization is shown in Fig.(5).

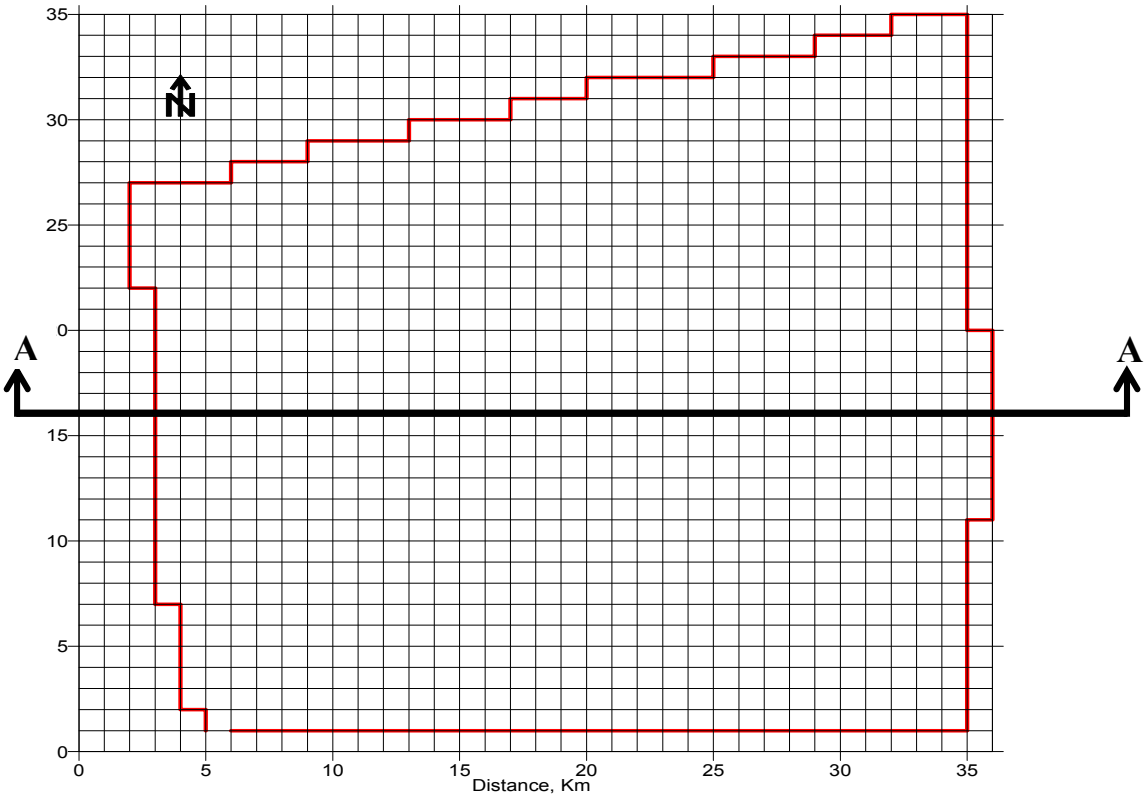

Fig.(5) Discretization Mesh Design of the model Domain

Base Map implementation :

The most important process is the adoption of the base map which is defined as *the number of cells in the model domain cover the boundary of the modeled area, and it is assigned in the modeling process by their individual xy coordinates as shown in table.(1)Appendix A.*

Data Input Files:

The following data are adopted for the proposed problem; they are specified by separated files for each node within the model domain:
D(I,J,1) = 1.5 m2/hr , D(I,J,2) = 0.2 m2/hr
V(I,J,1) = 1.2 m/hr , V(I,J,2) = 0.5 m/hr
, Delta = 0.2, Co = 1000 mg/l
The pollutant concentration of 1000mg/l is specified for the nodes along the west polluted boundary

Results & Discussion:

The model is run for long period and the induced concentrations are represented by the contour map of Fig.(6). The figure shows how the pollutant transports from the polluted boundary toward the river across a distance of 33km causing a concentration of 96 mg/liter at the river after a period of 905.6 days.

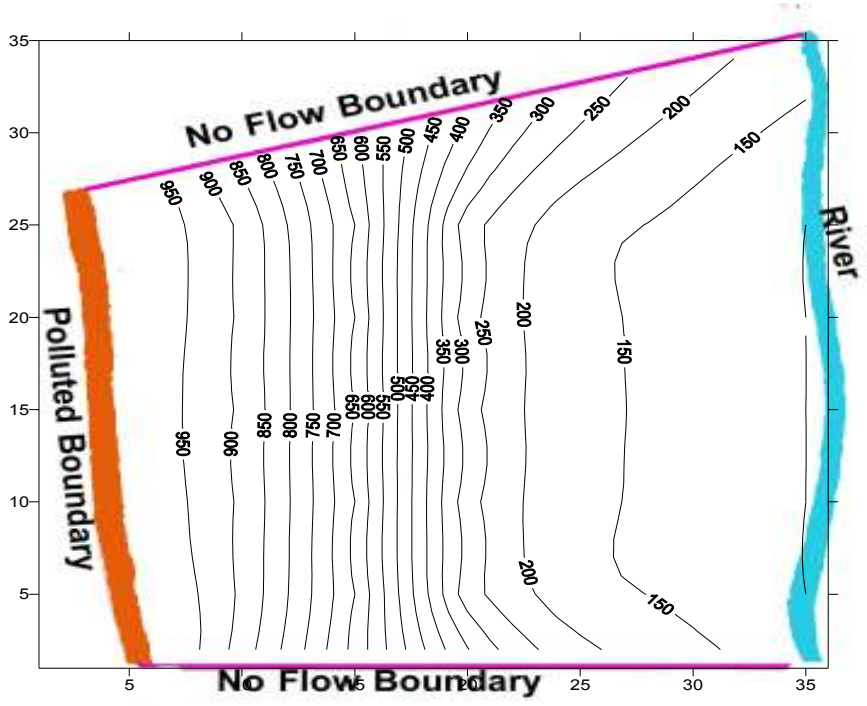

Fig.(6) Pollutant Distribution Contour Map in (mg/l)

Fig.(7) shows the concentration profile along section A-A which is shown in Fig.(5)

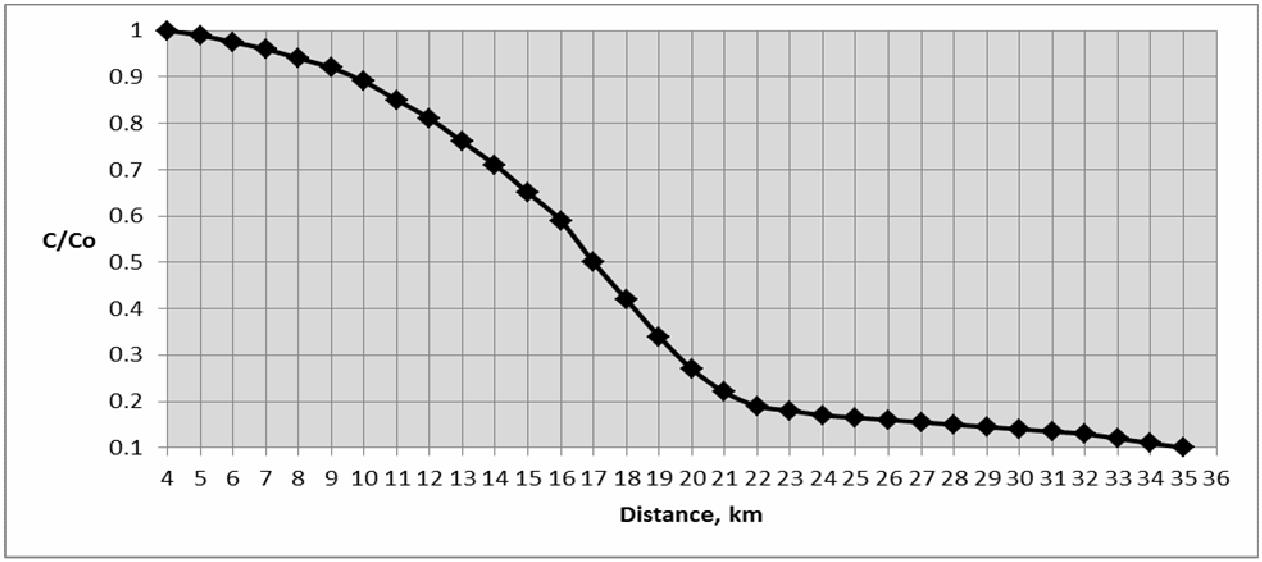

Fig.(7) Concentration Profile Along Section A-A

Conclusions:

The current technical study reveals the following conclusions:-

1- The current model has been proved to be a powerful tool to simulated and analyze any environmental disaster including; point, line and area pollution sources in subsurface saturated mediums.

2- The model can deal with a three dimensional subsurface systems by assigning the necessary data for each node within the model domain.
3- The undertaken problem has been analyzed by the current mathematical model and reasonable results are obtained.

Recommendations
It is recommended to:
1- Simulate the convection-dispersion problems of contaminant transport by using the current modeling technique.
2- Expand the current program to comprise the problems of pulses pollutants in groundwater media.

References:

1- Bear, J., "Some Experiments in Dispersion, Journal of Geophysical Research", Vol.66, No.8, pp.2455-2467, (1961).
2- Rumer R.R, "Longitudinal Dispersion in Steady and Unsteady Flow, Journal of Hydraulics Division", ASCE, Vol.88, HY4, pp.147-172, (1962).
3- Harleman D.R.F., and Rumer, R.R., "Longitudinal and Lateral Dispersion in an Isotropic Porous Medium", Journal of Fluid Mechanics, Vol. 16, Part 3, pp.385-394, (1963).
4- List, E.J., and Brooks, N. H., "Lateral Dispersion in Saturated Porous Media", Journal of Geophysical Research", Vol. 72, No. 10, pp.2531-2541, (1967).
5- Narasimhan, T.N., and Witherspoon, P.A, "Overview of the Finite Element Method in Groundwater Hydrology". Proceedings of the Fourth International Conference on Finite Elements in Water Resources, Hannover, Germany, (1982).
6- Smith I.M., Farraday, R.V., and O'Connor, B.A., "Rayleigh-Ritz and Galerkin Finite Elements for Diffusion-Convection Problems". Water Resources Research, Vol.9, No.3, pp.593-606, (1973).
7- Frind E.O., "The Principal Direction Technique: A New Approach to Groundwater Transport Modeling". Proceedings of the Fourth International Conference on Finite Elements in Water Resources, Hannover, Germany, (1982).
8- Peter Frolkovic and Jozef Kacur, "Semi-Analytical Solutions of Contaminant Transport Equation with Nonlinear Sorption in 1D". Federal Ministry of Economics and Technology (BMWi) under the contract number 02 E 9148 2, (2004).
9- Peter Knobloch, "Numerical Solution of Convection-Diffusion Equation Using Upwinding Techniques Satisfying the Discrete Maximum Principle". Proceedings of the Czech-Japanese Seminar in Applied Mathematics, Kuja Training Center, Oita, Japan, September 15-18, pp. 69-76, (2005).
10- Mirbagheri S. A., "Modeling contaminant transport in soil column and ground water pollution control" International Journal of Environmental Science & Technology, Vol. 1, No. 2, pp 141-1 50, Summer, 2004.
11- Prickett, T.A., and. Lonngquist, C. G., "Selected Digital Computer Techniques for Groundwater Resource Evaluation", (*Illinois State Water Survey Bulletin 55.)* pp 66, (1971).
12- Pinder, G. F., and Bredehoeft, J. D., "Application of the Digital Computer for Aquifer Evaluation",Water Resources Research, Vol.4, No. 5 Oct., pp. 1069-1083, (1968).
13- Erwin Kreyszig , "Advanced Engineering Mathematics", Published by John Wiley & Sons, Library of Congress Cataloque Card Number: 71-172951, (1972).

14- Peaceman D. W., Rachford H. H., "The Numerical Solution of Parabolic and Elliptic Differential Equation". Journal Society of Industrial and Applied Mathematics V.3: 23-41, (1955).

Appendix A

Table. (1) Base Map Design

Mesh No.	x	y	Mesh No.	x	y	Mesh No.	x	y	Mesh No.	x	y	Mesh No.	x	y
1	١	١	31	١١	٢١	61	٢٧	٢٥	91	٣٩	٧	121	٢٧	١
2	١	٢	32	١٢	٢١	62	٢٨	٢٥	92	٣٩	٦	122	٢٦	١
3	١	٣	33	١٢	٢٢	63	٢٩	٢٥	93	٣٩	٥	123	٢٥	١
4	٢	٣	34	١٢	٢٣	64	٣٠	٢٥	94	٤٠	٥	124	٢٤	١
5	٢	٤	35	١٢	٢٤	65	٣٠	٢٤	95	٤٠	٤	125	٢٣	١
6	٢	٥	36	١٣	٢٤	66	٣١	٢٤	96	٤١	٤	126	٢٢	١
7	٣	٥	37	١٣	٢٥	67	٣١	٢٣	97	٤٢	٤	127	٢١	١
8	٣	٦	38	١٤	٢٥	68	٣٢	٢٣	98	٤٣	٤	128	٢٠	١
9	٣	٧	39	١٤	٢٦	69	٣٣	٢٣	99	٤٤	٤	129	١٩	١
10	٤	٧	40	١٥	٢٦	70	٣٣	٢٢	100	٤٤	٣	130	١٨	١
11	٤	٨	41	١٥	٢٧	71	٣٤	٢٢	101	٤٥	٣	131	١٧	١
12	٤	٩	42	١٥	٢٨	72	٣٤	٢١	102	٤٥	٢	132	١٦	١
13	٥	٩	43	١٥	٢٩	73	٣٥	٢١	103	٤٥	١	133	١٥	١
14	٥	١٠	44	١٦	٢٩	74	٣٥	٢٠	104	٤٤	١	134	١٤	١
15	٦	١٠	45	١٦	٣٠	75	٣٦	٢٠	105	٤٣	١	135	١٣	١
16	٦	١١	46	١٧	٣٠	76	٣٧	٢٠	106	٤٢	١	136	١٢	١
17	٦	١٢	47	١٨	٣٠	77	٣٧	١٩	107	٤١	١	137	١١	١
18	٧	١٢	48	١٨	٢٩	78	٣٧	١٨	108	٤٠	١	138	١٠	١
19	٧	١٣	49	١٩	٢٩	79	٣٧	١٧	109	٣٩	١	139	٩	١
20	٧	١٤	50	١٩	٢٨	80	٣٨	١٧	110	٣٨	١	140	٨	١
21	٨	١٤	51	٢٠	٢٨	81	٣٨	١٦	111	٣٧	١	141	٧	١
22	٨	١٥	52	٢١	٢٨	82	٣٨	١٥	112	٣٦	١	142	٦	١
23	٩	١٥	53	٢١	٢٧	83	٣٨	١٤	113	٣٥	١	143	٥	١
24	٩	١٦	54	٢٢	٢٧	84	٣٨	١٣	114	٣٤	١	144	٤	١
25	٩	١٧	55	٢٣	٢٧	85	٣٨	١٢	115	٣٣	١	145	٣	١
26	٩	١٨	56	٢٤	٢٧	86	٣٨	١١	116	٣٢	١	146	٢	١
27	١٠	١٨	57	٢٤	٢٦	87	٣٩	١١	117	٣١	١			
28	١٠	١٩	58	٢٥	٢٦	88	٣٩	١٠	118	٣٠	١			
29	١١	١٩	59	٢٥	٢٥	89	٣٩	٩	119	٢٩	١			
30	١١	٢٠	60	٢٦	٢٥	90	٣٩	٨	120	٢٨	١			