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A Two Dimensional Flow and Transport Model for Tidally Influenced Aquifers

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Abstract. A 2D finite element model for predicting fate of soluble contaminants in confined or unconfined coastal aquifers has been developed. The influence of tidal effects on the groundwater flow and the pollutant transport process was a primary component of the model. The transport process modeling includes advection and dispersion. Attenuation mechanisms like adsorption and decay are not included in the model to make its estimates conservative. The main features of this model are its ability to represent the tidal boundary, and its capability of dealing with the nonlinearity resulting from variations in the saturated thickness in unconfined aquifers, and the new way of representing the general head boundary condition.

Introduction

It is well known that tides have some influence on the flow characteristics near the coast line. As expected, earlier studies have indicated that the tidal fluctuations cause some of the sea water to enter the aquifer at those times corresponding to a head gradient inland. Numerous numerical models of a general nature in which the effects of tidal fluctuations on groundwater flow dynamics and subsurface transport processes are not incorporated exist in the literature. Detailed information on such models are available in Mercer and Faust [1, 2, 3], and Faust and Mercer [4, 5]. Comprehensive reviews of available models are presented by Prickett [6], and Khondaker *et al.* [7].

Yim and Mohsen [8] presented a one-dimensional numerical model to simulate the migration process of a contaminant plume within tidally influenced aquifers, considering oscillating velocities and dispersions. They applied their simulation model to an ideal case assuming a sinusoidal boundary condition in a homogeneous and isotropic confined aquifer. Based on their simulation results, they concluded that tidal fluctuation causes the exit concentration levels to be significantly diluted by the surface water body of the estuary. They also performed a sensitivity analysis for the main influencing parameters which demonstrated that the tidal fluctuation hastened the rate of plume migration near the bank of the estuary because of the relatively high advective and dispersive fluxes induced by tides. However, tides affect the migration process only over the tidally active zone of the aquifer, the size of which depends on various aquifer parameters.

If the contaminated plume is located far beyond the interface, the tidal fluctuations will not affect the rate of plume migration until an existing regional groundwater velocity brings the plume to the tidally active zone. The rate of contaminant migration was found to increase with a higher regional hydraulic gradient irrespective of the tides.

No work has been reported in the literature on the study of tidal effects on flow and transport processes in unconfined aquifers, considering multi-dimensional flow with complex geometry, and boundary conditions. The objective of this study is to develop a numerical model capable of simulating two-dimensional unconfined aquifers with complex geometry and boundary conditions. Furthermore, spatial variations of the aquifer parameters have to be considered. Because of the complex nature of problems existing in the real world, a simple analytical solution for groundwater flow and/or one dimensional transport equation (as used by Yim and Mohsen [8]) can not be used to accurately simulate a field scale problem. Therefore, the resulting model should consider a coupled complex natural processes of simultaneous flow and transport of contaminants in the subsurface environment. The solution of such system requires application of advanced numerical techniques for both of the governing equations. The results obtained using such model will be more reliable than those predicted by a simplified one dimensional analysis.

Flow and Transport Equations

The governing partial differential equation for unsteady two dimensional flow in Cartesian coordinates is stated below:

$$\frac{\partial}{\partial x}\left(K_{xx}b\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}b\frac{\partial h}{\partial y}\right)+W=S_y\frac{\partial h}{\partial t} \tag{1}$$

where

K_{xx}, K_{yy}	are the hydraulic conductivities in x and y directions respectively,
h	is the hydraulic head,
W	is a source\sink term (representing recharge or discharge),
S_y	is the specific yield, and

b	is the saturated thickness of the aquifer.
t	time

It should be noted here that the saturated thickness h is a function of the head h in case of unconfined aquifers which makes the above equation nonlinear.

The governing partial differential equation for transient two dimensional solute transport is the advection-dispersion equation given below in global cartesian coordinates:

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j} - v_i C\right) + \frac{Q_p C^1}{\eta} = \frac{\partial C}{\partial t} \qquad (2)$$

where

c	is solute concentration,
D_{ij}	the hydrodynamic dispersion tensor,
V_i	the component of groundwater velocity in the i directions,
Q_p	source\sink term
c^1	is source concentration,
η	effective porosity.

In order to obtain a unique solution to a partial differential equation governing a certain physical process, additional information regarding the physical state of the process is required. This information is provided through the boundary and initial conditions.

Model Development

Finite element formulation of the governing equation in its general form is available in Voss [9, p. 95-122]. The resulting final equations obtained by the Galerkin finite element formulation are presented bellow.

$$[A_h]\,\{H\} = \{\Gamma_h\} \qquad (3)$$

$$[A_c]\,\{C\} = \{F_c\} \qquad (4)$$

where {H} and {C} are the vectors of nodal values of head and concentration respectively and the matrices ($[A_h]$ and $[A_c]$) and the vectors ($\{F_h\}, \{F_c\}$) are obtained through finite element formulation.

Solution Algorithm

Solution of the differential equations governing any physical system and/or phenomenon, is to find the unknown function that satisfy the governing equations with the associated boundary and initial conditions. The governing equations representing the natural system of groundwater flow and contaminant transport are coupled and hence needs to be solved simultaneously. However, at low contaminant concentrations the governing equation can be uncoupled allowing the flow equation to be solved first then using its solution in the transport equation. The nature of the nonlinearity should also be considered in solving these equations. The overall solution algorithm and the method of treatment of nonlinearities involved are presented in the following sections.

Solution of the governing equations

The simultaneous solution procedure of the governing equations (1) and (2) involves reading input data (Domain geometry, model parameters, initial condition) and select simulation mode (steady or unsteady), then solving the groundwater flow equation for the head distribution ($\{H\}$) from which the velocity and dispersivity fields are computed and used to solve the solute transport equation for contaminant concentration distribution. This procedure will be repeated for each time-step in transient simulation.

Treatment of nonlinearity in unconfined aquifers

As mentioned earlier, the groundwater flow equation (1) becomes nonlinear for the case of unconfined aquifer that demands an iterative solution schemes for the simultaneous determination of the water table position and the saturated thickness of the aquifer at different time horizons. A simple iterative scheme is used in this model. The iterative routine starts with an initial estimate of head distribution. Known (from observation) initial head distribution is normally used as the starting head values for both the steady and transient simulation. The groundwater flow equation using the saturated thickness obtained from the initial estimate of head distribution. After which the head distribution obtained is compared with the initial estimate. If the maximum difference between these values do not satisfy the required convergence criteria, the initial estimate of head values is updated using the new head distribution and re-solving the flow equation repeating this procedure until the convergence is achieved. This scheme has to be repeated for each time-step for the transient simulation where the initial estimate of the head distribution at a given time step was obtained from the previous time step.

Treatment of nonlinearity involved in GHB

The general head boundary condition (GHB) for the groundwater flow equation is given by

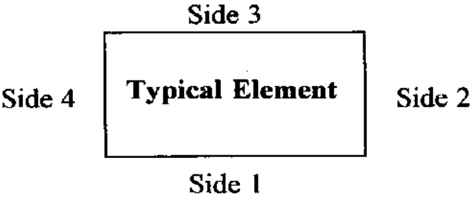
$$K_{xx}\frac{\partial h}{\partial x}l_x + K_{yy}\frac{\partial h}{\partial y}l_y = q \qquad (5)$$

where l_x and l_y are the direction cosines in x and y directions and q is the flux.
The general head boundary condition in the solution of groundwater flow equation can be treated by introducing time-dependent flux at the nodes on such boundaries. There are two approaches to define the time-dependent flux at the node:

1. Flux computed based on flow conditions inside the domain only
2. Flux computed based on flow conditions inside the domain and forcing a constant head condition outside the domain

The procedure for the first approach is discussed here. The nodal flux due to general head boundary can be calculated at anytime using the velocity field and the saturated thickness at that time. The sign conventions for the flux q are shown in Fig. 1. The total flux through each side of the element on general head boundary were calculated using the following expressions:

Side - 1 $$F_T = \eta A_x V_{yy} \quad (6)$$



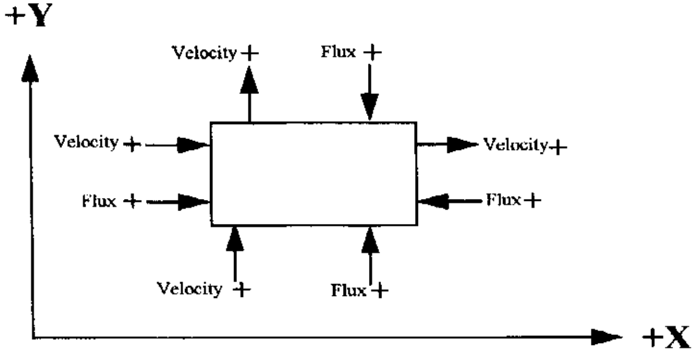


Fig. 1. Sign conventions for the flux due to general head boundary condition.

where

A_x flow area = $T_{sat} L_e$
F_T total flux along side,
T_{sat} saturated depth at element centroid,
L_e side length.

Similar expressions for the total flux through the other sides can be obtained.

The nodal values of the flux due to general head boundary condition can be obtained assuming equal distribution of the total flux between the two nodes on that side.

Since the flux on the general head boundary depends on the head gradient which is not known at beginning of the solution procedure, the resulting finite element equation for groundwater flow becomes nonlinear that needs to be solved iteratively. In case of unconfined aquifer, the nonlinearity increases because the saturated thickness (T_{Sat}), which is a function of head, is also unknown at the beginning of the solution.

The iterative scheme involves solving the groundwater flow equation with the given initial condition assuming no flux at the general head boundary nodes then updating the initial head distribution and calculating the nodal flux for the nodes on the general head boundary using equation (6) with the head distribution obtained. Also the saturated thickness is calculated if the aquifer is unconfined. The groundwater flow equation is then solved using the updated values of head distribution and the nodal flux and saturated thickness (only for unconfined aquifers). The head distribution obtained is compared with the initial values. If the maximum difference does not satisfy the required convergence criteria the initial estimate of head values, nodal flux and saturated thickness (only for unconfined aquifers) are updated using the new head distribution. This process is repeated until the convergence is achieved. This iterative scheme is repeated for each time-step for transient simulations where the initial estimate of head distribution at a given time-step was obtained from the previous time step.

It is worth mentioning that this procedure for the treatment of general head boundary conditions can not be used for the steady state simulation.

Initial conditions

The initial conditions are the starting values of the primary variables (i.e. head and concentration in equations (1) and (2) respectively), which are necessary for nonlinear and transient simulations, and generally obtained from collected data and field investigations.

Boundary conditions

A combination of specified head, time-dependent head and general head were used for the groundwater flow equation. The time-dependent head boundary conditions is somewhat similar to the cyclic tidal values given by the tidal data. For the transport boundary conditions, a technique similar to the one given by Yim and Mohsen [8] was used to supply the concentration boundary values. This technique involves specifying different boundary conditions, depending on the prevailing flow direction at the time of analysis (whether flow is from or towards the sea).

Computer Codes

Computer implementation of the solution algorithm for the resulting governing equations involves the design of model structure and the development of various codes using suitable computer languages. The final result is a modeling package called CONTRANS. This package consists of two main components, the numerical simulator, which contains a number of subroutines developed using Microsoft FORTRAN Power Station to implement the solution algorithm for the governing equations, and the input-output processor which is made user friendly using Microsoft Visual Basic (Version 3.0) to develop a Windows based Graphical User Interface (GUI). The overall structure of the model is shown in Fig. 2. A detailed manual covering the package development details is available from the authors.

Model Testing and Application

Three sample problems are presented in this section with the objectives of validating the predictions of the developed computational model (case 1), and demonstrating the ability of this model to handle more realistic type problems (case 2 and 3). The detailed input data for the three cases are given in the Table. Case 1 involves a steady one dimensional flow and transport between two reservoirs on which the head and concentration values are fixed. The finite element grid used to simulate this problem is shown in Fig. 3. The analytical solutions for the head and concentration distribution are obtained by solving equations 1 and 2 for this simple case and using the appropriate boundary conditions for the head and the concentration which yield the following equations:

$$h^2(x) = h_o^2 - \frac{(h_0^2 - h_L^2)}{L} X \tag{7}$$

$$c(x) = C_o - \frac{1-\exp\left(\frac{L}{\alpha_L}\right)}{C_o - C_L} + \frac{1-\exp\left(\frac{L}{\alpha_L}\right)}{C_o - C_L} \exp\left(\frac{X}{\alpha_L}\right) \tag{8}$$

where

h_0 the head value at x=0,

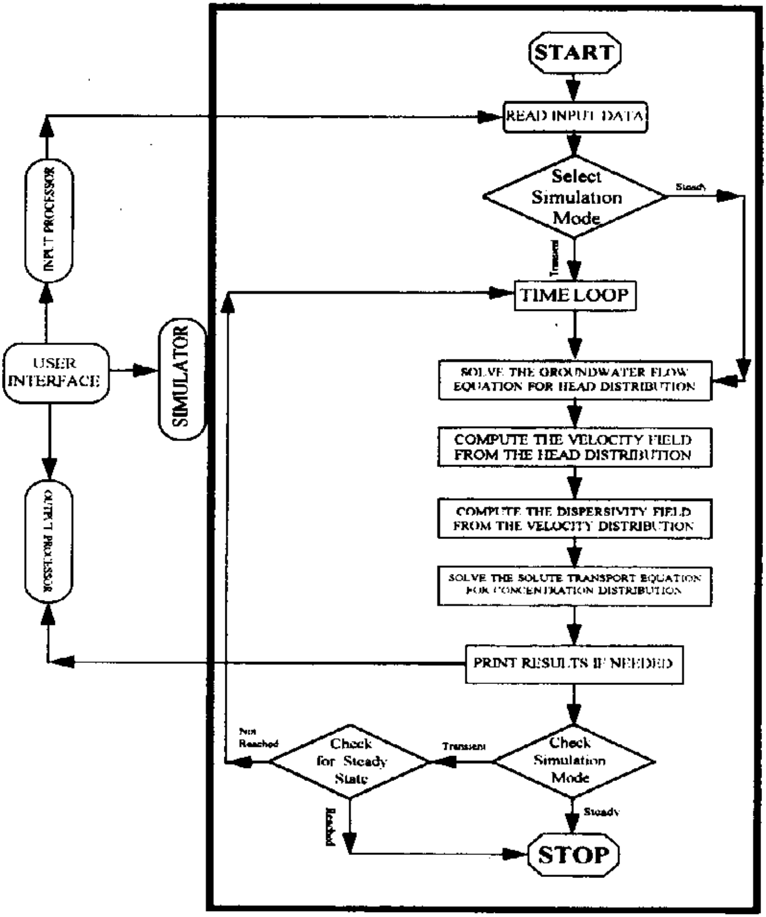


Fig. 2. Contrans structure.

h_L the head value at x=L

c_0 the concentration at x=0

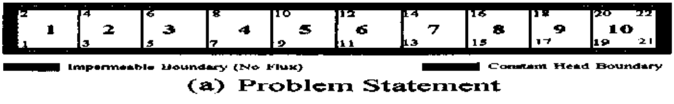
c_L the concentration at x=L

a_L the longitudinal dispersivity

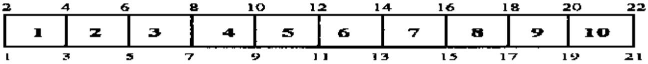
L total flow length.

Table. Input data for test problems

Input data	Case 1	Case 2	Case 3
Domain area	10m x 10m	100m x 60m	100m x 60m
Δx	10m	10m	10m
Δy	10m	10m	10m
NE	10	60	60
NN	22	77	77
Flow condition	Steady	Transient	Transient
Transport condition	Steady	Transient	Transient
Aquifer type	Unconfined	Confined	Confined
Hydraulic conductivity	0.7 m/day	0.7 m/day	0.7 m/day
Aquifer thickness	Variable	10m	10m
α_L	10m	10m	10m
α_T	1m	1m	1m
Boundary conditions			
Nodes	1-2 21-22	1-7 other	1-7 other
Head	11 10	11 tidal	11 tidal
Concentration	1000 0	1000 0	1000 0
Solute source nodes	None	None	32,38,39,40



(a) Problem Statement



(b) Finite element Grid showing Node and Element numbers

Fig. 3. (a) Problem statement; (b) Finite element grid showing node and element numbers.

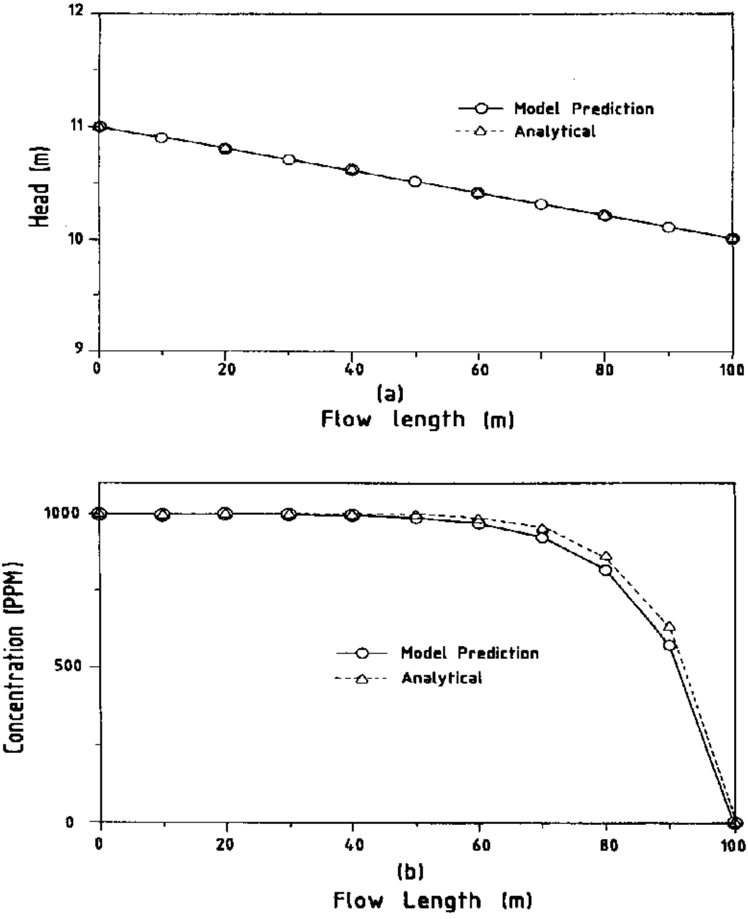
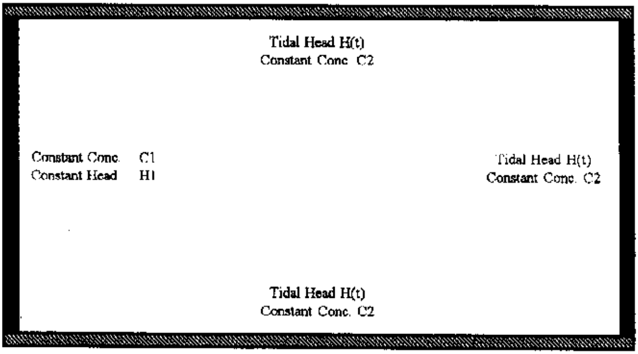
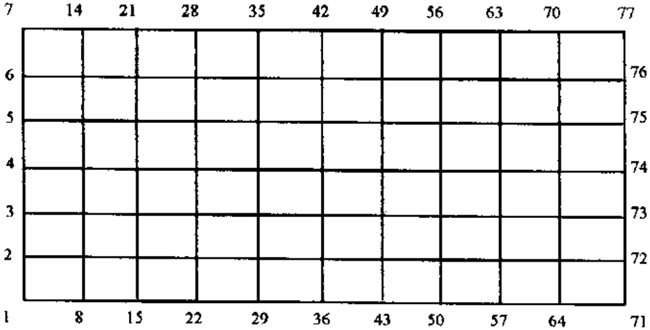


Fig. 4. Comparision between model predictions and analytical solutions for case 1.



(a) Geometry & Boundary Conditions



(b) Finite element Grid showing Boundary nodes

Fig. 5. (a) Geometry and boundary conditions; (b) finite element grid showing boundary nodes.

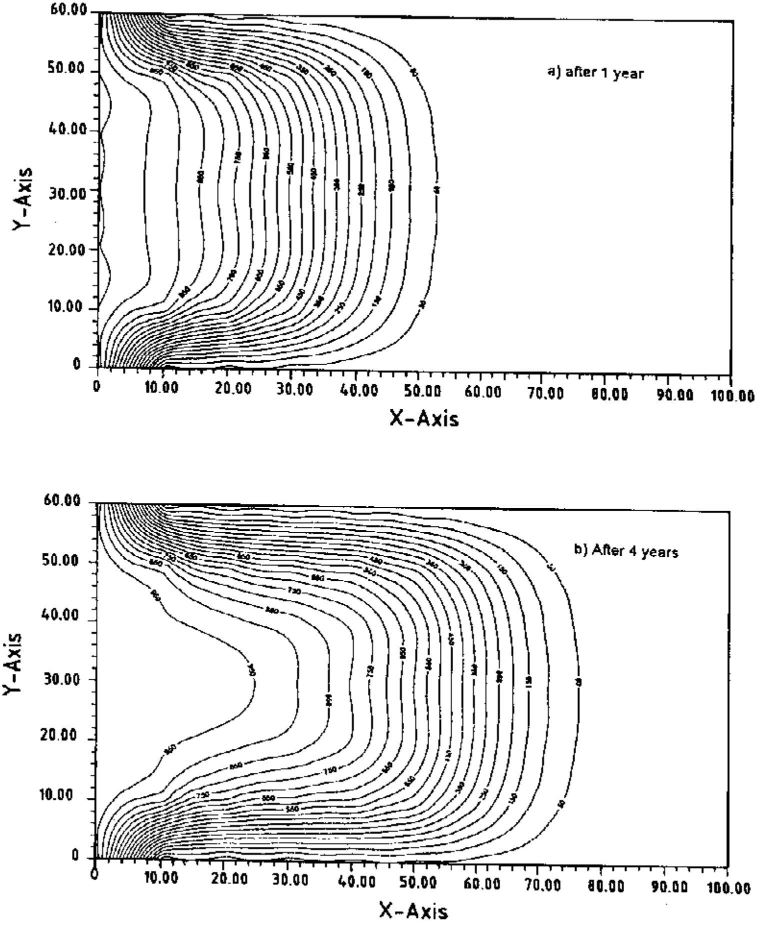
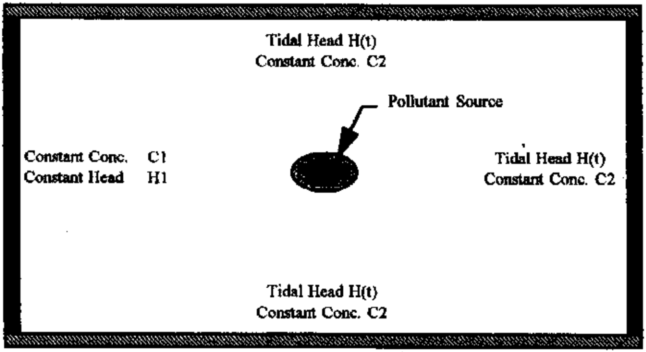
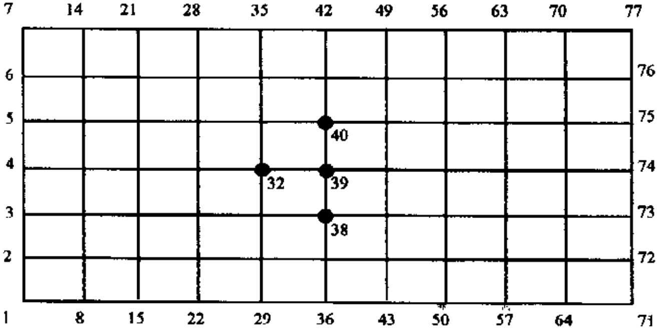


Fig. 6. Model predicted concentration for case 2.



(a) Geometry & Boundary Conditions



(b) Finite element Grid showing Boundary and Source nodes

Fig. 7. (a) Geometry and boundary conditions; (b) Finite element grid showing boundary and source nodes.

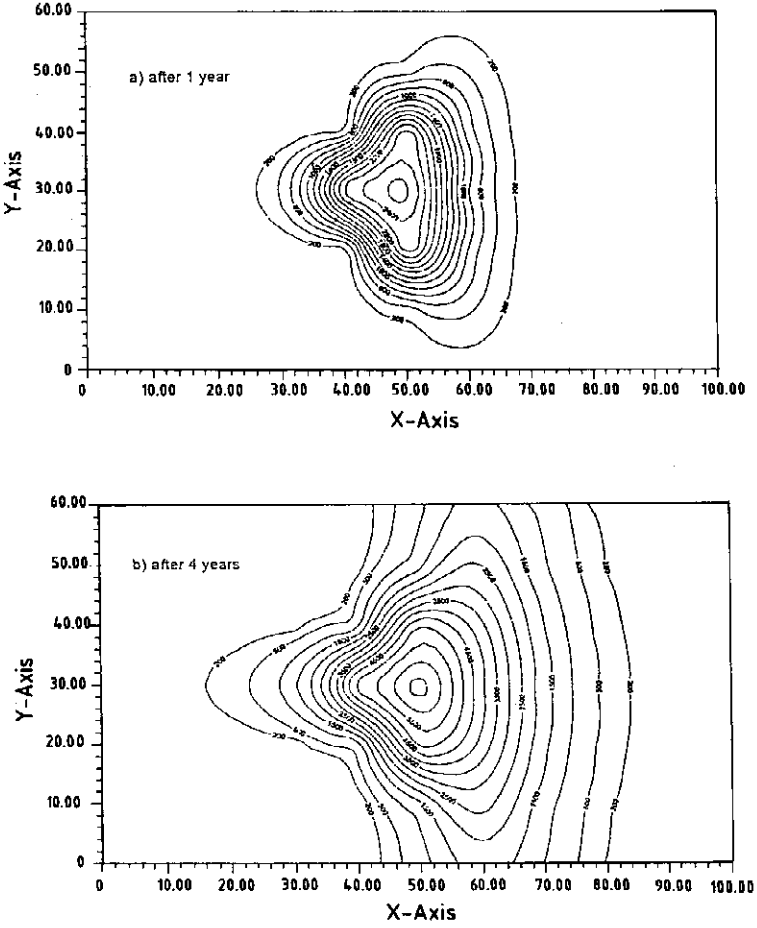


Fig. 8. Model predicted concentration for case 3.

The results for the head and concentration along the flow length are given in Fig. 4 in which the model predictions are compared with the analytical solution. Figure 4.a shows an excellent agreement between predicted and exact values for head. Figure 4.b shows good agreement between the two solutions with a small deviation at the region of very high concentration gradient. Such deviation can be reduced by choosing a relatively smaller grid size.

Cases 2 and 3 are presented to demonstrate the ability of the model to represent the tidal boundary condition as well as the contamination source. Case 2 deals with the transient flow and transport in a confined aquifer with three sides subjected to tides and a constant head at the forth. The tidal boundary condition is approximated by the superposition of an average head value and a sine function with a period of half a day and an amplitude of one meter. The finite element grid and the concentration distribution after one and four years are given in Figs. 5 and 6. Case 3 is similar to case 2 except that a contaminant source is introduced near the center of the aquifer. This problem could represent a simplified form of the transport of dissolved organic contaminants due to a leaking petroleum storage tank in a coastal area. The problem geometry and the predicted contaminant plumes after 1 and 4 years are shown in Figs. 7 and 8.

Summary

A two dimensional finite element areal simulation model was developed to model the flow and contaminant transport in porous media. This model, **CONTRANS**, simulates the flow and transport of soluble contaminants due to advection, diffusion and mechanical dispersion. The developed algorithm ensures the preservation of the non-linearity in the governing equations for the cases of unconfined flow and time dependent flux. It also has the unique ability to represent the tidal boundary condition which is important in studying contaminant transport in coastal aquifers. **CONTRANS** has been made powerful and user friendly through the windows based Graphical User Interface that enables any professional without any knowledge of programming to apply this model effectively.

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نموذج ثنائي الأبعاد لعملية الجريان والنقل في الخزانات الجوفية المتأثرة بحركة المد والجزر

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(استلم في ٣/٧/١٩٩٦م ؛ وقُبل للنشر في ٢٨/١٢/١٩٩٦م)

ملخص البحث. طور نموذج ثنائي أبعاد باستخدام طريقة الأجزاء المحددة بغرض تقدير تركيز الملوثات الذائبة في خزانات المياه الجوفية الساحلية بنوعيها، المحصورة وغير المحصورة. إن تأثير حركة المد والجزر على جريان الماء وعملية نقل الملوثات أهم أهداف هذا النموذج. تم تمثيل عمليات نقل الملوثات بظاهرتي الجريان والانتشار. ولكي تكون تقديرات النموذج متحفظة فقد تم استبعاد العمليات الإبطائية مثل الامتصاص والتلاشي. إن أهم خصائص هذا النموذج قدرته على تمثيل مختلف الظروف المحيطة بما فيها حركة المد والجزر وقدرته على التعامل مع المعادلة غير الخطية والناتجة عن تغير مساحة الجريان في الخزانات الجوفية غير المحصورة.