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A finite element program for groundwater pollutant transport and simulation

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Abstract
Groundwater, once believed to be the purest water source on earth, has been now contaminated as a result of rapid industrialization and other human activities in most parts of the worlds. Management of the groundwater systems requires a detailed understanding of the response of the aquifer under the imposed conditions. Due to non-linear and non-analytical nature of the pollutant transport model, numerical methods are must for solving the problem. In this research work, a model for groundwater pollutant transport has been formulated using Galerkin finite element numerical method. Using this formulation of the model an FEM program has been developed. The model is applicable for nonhomogeneous and unisotropic aquifer with irregular boundaries and single conservative pollutant. The use of the model has been demonstrated with the help of two case studies. The success of the model shows that the developed program can be used as a tool to solve the problems directed towards the management for groundwater resources.

INTRODUCTION

The finite element method is a numerical technique commonly used for the solution of groundwater flow and mass transport problems. For any groundwater problem the finite element method is superior to classical finite difference models. Medium heterogeneity and irregular boundary conditions are handle naturally by the finite element method (FEM). This is the contrast to difference interpolation schemes, which at the best approximate the complex boundary conditions. More over, in the finite element method, the size of the element can be easily varied to reflect rapidly changing state variables as well as the parameters of groundwater system which also increase the accuracy of the numerical approximation (Bear and Veeriujit, 1987).

The finite element method has evolved with the ready availability of high-speed electronic digital computers and increasing emphasis on numerical methods for engineering analysis. In finite element method, instead of solving the problem for the entire body in one operation, the solutions are formulated for each constituent unit and finally combined to obtain the solution for the original body. Although the analysis procedure is thereby considerably simplified, the amount of data to be handled is dependent upon the number of smaller bodies (elements) into which the original body is divided. For a large number of subdivisions, it is a formidable task to handle the volume of data manually and hence a high speed digital computer is a must to solve the problem.

A number of computer packages have been developed for solving groundwater pollution problem. Some of them are SOLUTE (Bleyin, 1985), SEFTRAN (Huyakorn et al., 1989) etc. But they are not easily available and are designed for solving particular problem only.

In the present research a set of tools for solving groundwater flow (GWFM) and pollutant transport (GWPTM) have been developed. Both GWFM and GWPTM models are meant for general purpose and are capable of solving any two dimensional groundwater problem in aquifer with any geometry or irregular shape and for all three types of boundary conditions being imposed anywhere in any form. The models have the capability of automatic mesh generation for regular right-angled triangular element. However, it is possible to directly input the node numbers and coordinates of triangular elements of any shape and size. The GWFM model may be used as a module to run any other specific groundwater pollution problem. This set of tools could be used to identify cleanup strategies. However no optimization procedure has been included. Both the models are written in FORTRAN 77 and implemented in UNIX operating system. The code is successfully run and tested using DEC AXE 3000 system at IIT, Kharagpur.

FEM FORMULATION

Unsteady Flow in Aquifers

The basic partial differential equation for an isotropic aquifer (Bear and Veeriujit, 1987) is given by

$$S\frac{\partial \Phi}{\partial t}=\frac{\partial}{\partial x}\left(T\frac{\partial \Phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial \Phi}{\partial y}\right) \tag{1}$$

where S is the storativity, T is coefficient of transmission, and ϕ is head potential.

The boundary conditions are (1) head at any position along boundary, (2) rate of pumping or recharge at any point, along the boundary. The initial condition is written as

$$t = 0 \; ; \; \Phi = \Phi^0 (x, y) \tag{2}$$

where Φ^0 (x, y) is a known function.

The problem is solved by stepwise integration in time. A procedure will be developed in which the value at the end of a time step can be obtained starting from the initial values. For next time step can be made by considering the value at the end of the first time step will be treated as the initial value for the second step and so on. A simple way of deriving the basic algebraic equation of the numerical manhood is to integrate the differential equation 1 from t = 0 to t = Δt

$$S\frac{\Phi^{'}-\Phi^{0}}{\Delta t}=\frac{\partial}{\partial x}\left(T\frac{\partial \Phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial \Phi}{\partial y}\right) \tag{3}$$

where Φ' is the value of the head at the end of the time interval has been considered Δt.

While the value of Φ is average over time interval Δt. They are obtained by integrating over Δt and dividing the result by Δt can be expressed in terms of head at beginning and at the end of the time interval in the following form

$$\Phi = \varepsilon\, \Phi^0 + (1-\varepsilon)\, \Phi^{'} \tag{4}$$

where ε is an interpolation constant between 0 and 1.

Equation 4 states that the average value is linear combination of the initial value and the final one. In terms of finite differences, this would lead to the Crank-Nicholson scheme. From eq. 4

$$\Phi^{'} - \Phi^0 = \frac{\Phi - \Phi^0}{1-\varepsilon} \tag{5}$$

So equation 3 may be rewritten as

$$\frac{\partial}{\partial x}\left(T\frac{\partial \Phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(T\frac{\partial \Phi}{\partial y}\right) - \frac{S(\Phi^{'} - \Phi^0)}{\Delta t(1-\varepsilon)} = 0 \tag{6}$$

In finite eliminate method, the region R in which the flow takes place is subdivided into a large number of small elements, in each of which the ground water flow is approximated by some simple function. The simplest way of subdividing the region is by using triangular elements. Such elements make it possible to closely follow natural boundaries. The values of heads to be determined at the nods of all elements. The simplest way of approximating the variation of the within a triangular element is to assume that the head varies linearly within each element. The piezometric surface is thus approximated by diamond shaped surface as in each element the head is represented by a planner surface. The ground water head at a point inside an element is defined by a linear interpolation between the values at the nodes.

Using notion of FEM, the piezometric head Φ through the entire region can be expressed by

$$\Phi = \sum_{j=1}^{n} N_j(x, y)\Phi_i \tag{7}$$

where Φ_i is the head at the node i, and N_j is the shape function, or basic function, defined by $N_j = 1$ if $j = i$, and $N_j = 0$ for $j \neq i$.

In general, the approximation will not exactly satisfy the partial differential equation (eq. 6). Therefore the condition is by requiring the differential equation be satisfied only on average, using a number of weighted functions equal to number of unknowns. This is called method of weighted residuals. Here Galerkin approach is used i.e., shape function N_J are used as weighted functions. This leads to the conditions from theory of FEM to be satisfied for each node i for whichΦ_I is unknown. By satisfying Eq. 8 for all nodes i in the problem domain, a set of algebraic equation is obtained. The number of equations is equal to number of unknown values.

$$\int_R \left(\left(\frac{\partial}{\partial x}\left(T\frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y}\left(T\frac{\partial \Phi}{\partial y} \right) - \frac{S(\Phi' - \Phi^0)}{\Delta t(1-\varepsilon)} \right) N_j \right) dxdy = 0 \tag{8}$$

Eq. 8 can be written in matrix form as

$$\sum_j \left(P_{ij}\Phi_j + R_{ij}(\Phi_j - \Phi_j^0) \right) = Q_j \tag{9}$$

Pollutant Transport

In this section, a finite element model for the two-dimensional advective, dispersion problem is presented (Bear and Veeriujit, 1987; Bredehoeft et al., 1973). The basic differential equation to be solved is

$$n\frac{\partial C}{\partial t} = -V_x\frac{\partial C}{\partial x} - V_y\frac{\partial C}{\partial y} + \frac{\partial}{\partial x}(D_{xx}\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D_{yy}\frac{\partial C}{\partial y}) - Q(C - C_0) \tag{10}$$

where V_x and V_y are velocities in x and y directions respectively. The velocity vector is defined as

$$V = k \nabla \Phi \tag{11}$$

where k are the coefficients of permeability.

The average value of C is assumed to be given by the interpolation formula

$$C = \alpha C_0 + (1- \alpha) C' \tag{12}$$

where α is an interpolation parameter.

Substituting eq. 12 into eq. 10,

$$-V_x\frac{\partial C}{\partial x} - V_y\frac{\partial C}{\partial y} + \frac{\partial}{\partial x}(D_{xx}\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D_{yy}\frac{\partial C}{\partial y}) - Q(C - C_0) - \frac{n(C - C_0)}{(1-\varepsilon)\Delta t} = 0 \tag{13}$$

The assumptions for finite element method used in groundwater flow are also applicable to mass transport equation. The physical variables (the piezometric head Φ and the pollutant concentration C) are defined at the nodes of a network of triangles and the linear interpolation in the element is performed by the definition of shape function N_I (x, y), such that

N_I = px + qy + r
$N_I(x,y) = 1$ if $x = x_I$, $y = y_I$
$N_I(x,y) = 0$ if $x = x_j$, $y = y_j$ or $j \neq I$

The concentration C can be expressed as

$$C(x, y, t) = \sum_{j=1}^{n} N_j(x, y) C_i$$

The velocity, which is defined as the derivative of the head, is constant through out each element. The velocity distribution can be as a separate problem, independent of the solution for concentration. In other words, the two problem determining Φ (x,y,t) and determining C (x,y,t) are uncoupled. Accordingly, it is assumed that the groundwater flow problem has been solved and that the velocity components in all elements can be considered as known.

The finite element equation can be derived by the Galerkin approach. This means, that the partial differential equation 13 is multiplied by each of the shape functions and the result is integrated over the domain R. Each of the surface integrals can be evaluated by a summation of integrals over the triangular elements. For evaluation of the integral over a single triangle, the basic equation can be written in the form

$$\int_{R_p} (N_i(-V_x \frac{\partial C}{\partial x} - V_y \frac{\partial C}{\partial y} + \frac{\partial}{\partial x}(D_{xx}\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D_{yy}\frac{\partial C}{\partial y}) - Q(C - C_0) - \frac{n(C - C_0)}{(1-\varepsilon)\Delta t}))dxdy = 0 \qquad (14)$$

where R_p is the area of element number p. The summation of the J_p on all elements should be zero.

$$\sum_{p=4}^{m} J_P = 0 \qquad (15)$$

The first two terms of the eq. 15 can be separated into two parts by noting that

$$-D_{xx}\frac{\partial N_i}{\partial x}\frac{\partial C}{\partial x} - D_{yy}\frac{\partial N_i}{\partial y}\frac{\partial C}{\partial y} + \frac{\partial}{\partial x}(D_{xx}\frac{\partial C}{\partial x}) + \frac{\partial}{\partial y}(D_{yy}\frac{\partial C}{\partial y})N_i - \frac{\partial}{\partial x}(N_i D_{xx}\frac{\partial C}{\partial x}) - \frac{\partial}{\partial y}(N_i D_{yy}\frac{\partial C}{\partial y}) \qquad (16)$$

By substituting the above terms in eq. 15 and solving, it yields the following matrix equation

$D_{ij}\ C_j + E_{ij}\ (C_j - C_0) = 0$

where C_0 is initial concentration vector and C_j is concentration after time step Δt.

From the above equation, the unknown values of C_j can be found.

DEVELOPING FEM COMPUTER PROGRAM

As mentioned earlier the solution of the pollutant transport problem is written in two parts, one is for solving groundwater flow (GWFM) and second is for solving pollutant transport (GWPTM). Thus, the velocity components in the mass transport equation are calculated using first model (GWFM). In other words, the models are uncoupled. Because of computer codes in the literature are coupled. Since uncoupled models, the model developed for groundwater flow problem can also be used for other problems in environmental engineering such as water supply, groundwater cleanup programs etc.

As mentioned earlier the first step in the FEM is to discretize the continuum into small elements. For this purpose a computer code is written to generate regular right-angled triangular elements for regular shape of continuum. This automatic mesh generation is useful for the problems, which are having regular boundaries. This automatic mess generation code can also take care of any irregular shape of continuum, provided the values of node numbers, their coordinates and the nodes corresponding to each element, have been directly specified.

Groundwater Flow Model

Computer code is written for two dimensional, vertically averaged flow. This program can be solved any groundwater flow problem with steady state or unsteady state condition. Inputs parameters such as pumping or recharge are to be specified at nodes only.

The algorithm for groundwater flow model is as follows:

Read the coordinates of each node. Read dependent variables such as S, T, etc. and discharge at nodes if any.

For element m and corresponding nodes convert the co-ordinates x, y into local co-ordinate system.

Calculate 3x3 matrices p_{lk} and r_{lk} as follows for l = 1,2,3 and k = 1,2.3

$$p_{lk} = (T/2)A(b_l b_k + c_l c_k)$$

$$r_{lk} = \frac{(b_l b_k Z_{xx} + b_l b_k Z_{yy} + (b_l c_k + b_k c_k)Z_{xy} + d_l d_k)}{2A\Delta t(1-\varepsilon)}$$

where

$b_1=y_2-y_9$	$b_2=y_9-y_1$
$b_9=y_1-y_2$	$c_1=x_9-x_2$
$c_1=y_1-y_9$	$c_9=x_9-x_1$
$d_1=x_2y_9-x_9y_2$	$d_2=x_9y_1-x_1y_9$
$d_9=x_1y_2-x_2y_1$	
$Z_{xx}=(x_1^2 + x_2^2+x_9^3)$	
$Z_{yy}=(y_1^2 + y_2^2+y_9^3)$	
$Z_{xy}=(x_1y_1 + x_2\ y_2+x_9\ y_9)$	

Store the values of p, r at appropriate place in global matrices P and R respectively.

Repeat the above steps 3,4 for all elements.

Read initial and boundary conditions.

Convert the matrix equation

$P_{ij}\ \Phi_j + R_{ij}\ (\Phi_j - \Phi_j^0) = Q_j$ into $a_{ij}\ \Phi_j = b_j$

The above equation is solved for unknowns using any standard matrix method or iteration method for linear equations. Gauss-sidel over relaxation method is used for the solution of above equation.

Repeat the step 7, 8 for different time steps. For steady state flow, R_{ij} = [0].

Groundwater Pollutant Transport Model

Computer program GWPTM for groundwater pollutant transport is written for two dimensional, vertically averaged, confined aquifer system. For calculating the velocities in each element, it will use the values of heads calculated by groundwater flow model GWFM. This model is applicable for conservative pollutant, only.

The algorithm used is as follows:

Read the values of co-ordinate of each node, and nodes corresponding to each element. Read the values of heads at all nodes as calculated by groundwater flow model GWFM, read source and sinks also.

For element m and corresponding nodes, convert the global co-ordinates into local co-ordinates.

Calculate element velocity in the element as follows

$$\begin{bmatrix} V_x \\ V_y \end{bmatrix} = K/(2A)\begin{bmatrix} c_1 ... c_2 .... c_9 \\ b .... b ..... b \end{bmatrix}\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix}$$

$$K = \begin{bmatrix} K \;....0....0 \\ 0.....K_y....0 \\ 0.......0......K_z \end{bmatrix}$$

Calculate the total velocity V = $\sqrt{}$ $(V_x^2 + V_y^2)$, and calculate D_{xx} , D_{xy} , D_{yy}.

Calculate matrices p_{lk} , f_{lk} and r_{lk} as follows for l = 1, 3 and k = 1, 3

$$p_{lk} = \frac{(b_l b_k D_{xx} + b_l b_k D_{yy} + (b_l c_k + b_k c_k) D_{xy_k})}{2A}$$

$$r_1 = \frac{(b_l b_k Z_{xx} + b_l b_k Z_{yy} + (b_l c_k + b_k c_k) Z_{xy} + d_l d_k)}{2A} n$$

F_{lk}= A/6(V_x(b_l+b_k)+V_y(c_1+c_k))

$$r_2 = \frac{r_1}{\Delta t(1-\varepsilon)}$$

r_3 = Q * r_l

r_{lk} = r_2 + r_3

Store the matrices p_{lk} , f_{lk} and r_{lk} at appropriate place in global matrices P_{ij} , F_{ij} and R_{ij}.

Continue the step 2 to 6 for all elements.

Read boundary conditions and initial conditions of the problem

Convert the matrix equation
$P_{ij} C_j + F_{ij} C_j + R_{ij} (C_j - C_j^0) = 0$ into the form $a_{ij} C_j = b_j$.

Above equation is solved for unknown vector C_j, concentration after time step Δt, using Gauss-Sidel method.

USING THE PROGRAM

Case Study 1

To solve a typical groundwater flow problem, a square aquifer of dimensions of 1400 m x 1400 m has been chosen for which analytical solution is known. The confined aquifer is isotropic, and homogeneous. The aquifer has two impervious boundaries AB and DC, and two constant head boundaries AD and BC. The values of constant head along the boundaries AD and BC is assumed to be 100 m. The pumping well is located at the center of the aquifer.

The numerical solution of this problem is obtained using GWFM developed in this research. The area is divided into 225 nodes and 392 elements, the finite element mesh is shown in the figure 1. The parameters have been taken as Δx = 100 m, Δy = 100 m, Δt = 1 day, Q = 10000 m^3/s, S = 0.001, and T = 100 m^2/s. Initial and boundary conditions used are Φ (x, y, 0) = 100 m, Φ (0, y, t) = 100 m, Φ (1400, y, 0) = 100 m, q (x, 0, t) = 0.0 m^2/s and q (x, 1440, t) = 0.0 m^2/s.

Different numerical runs are made with GWFM model. The results are compared with analytical solution given by Willis and Yeh (1983). Table 1 shows the comparison between analytical and model results. The order of magnitude of difference between model and analytical results is less than 1% for the mesh size of 100 m x 100 m and less than 0.1% for mesh size 50 m x 50 m (results table not included here).

Table 1. Comparison of analytical and model results for case study 1

Node no	X (m)	Y (m)	Solution after 1 day		Solution after 10 day		Steady state solution	
			Analytical	Model	Analytical	Model	Analytical	Model
1	0	0	100.00	100.00	100.00	100.00	100.00	100.00
17	100	100	99.565	99.495	97.013	97.065	96.984	96.999
33	200	200	98.863	98.834	93.804	93.907	93.746	93.779
49	300	300	97.538	97.789	90.095	90.252	90.013	90.066
65	400	400	95.027	95.946	85.451	85.672	85.349	85.437
81	500	500	90.271	92.381	78.983	79.313	78.864	79.042
97	600	600	80.362	84.376	67.953	68.720	67.825	68.426

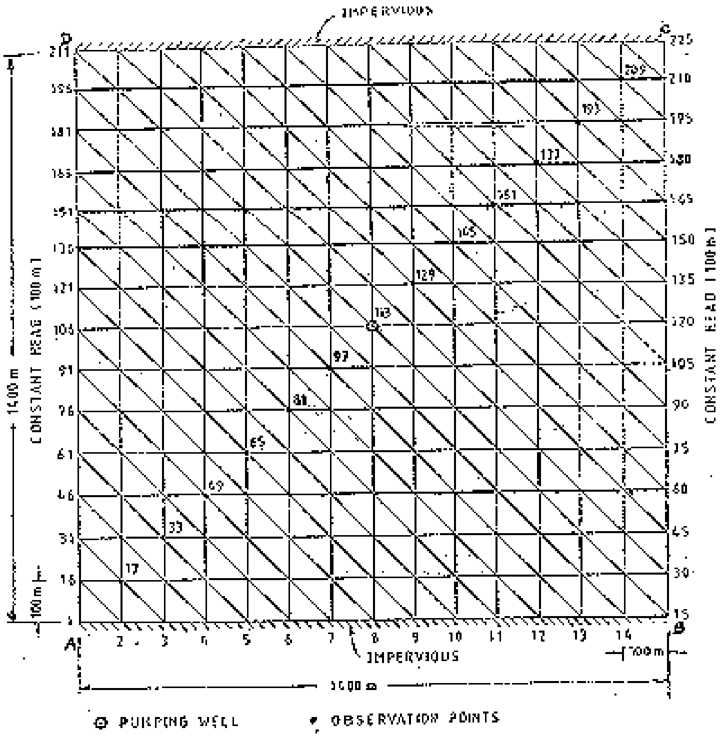

Figure 1. Finite element mesh and boundary conditions for case study 1.

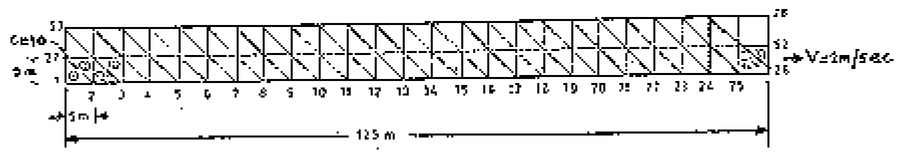

Figure 2. Finite element mesh for case study 2.

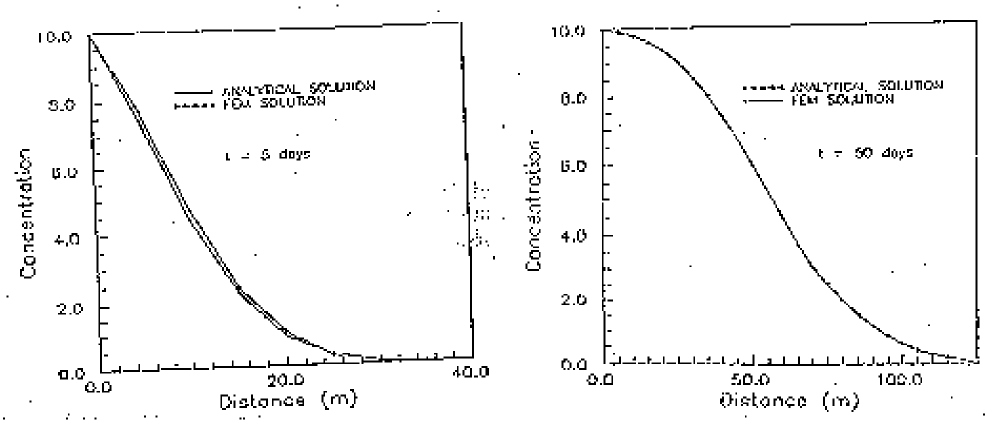

Figure 3. Typical performance of model for case study 2.

Case Study 2

The case study is for the movement of a tracer in a semi-infinite column. The governing equation for this case us written as

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x}$$

where D is longitudinal hydrodynamic dispersion coefficient and V is average pore water velocity.

Appropriate initial and boundary conditions for the problem considered are C (x,0) = 0, C ($\propto$,t) = 0 and C (0,t) = C_0.

The analytical solution to the above problem is well known and is given by

$$C(x,t) = C_0 / 2(erfc(x - vt) / 2(Dt)^{0.5} + \exp(Vx / D)erfc(x + vt) /(2(Dt)^{0.5})$$

Figure 2 shows the finite element mesh used for the problem. A total of 76 nodes and 100 two-dimensional triangular elements were used to simulate this problem, which is enough to represent the semi-infinite region in the given time interval ($0 \le t \le 50$). The only reason to use three modes along the Y direction is to maintain symmetry. The parameters used are as Δx = 5 m, Δy = 5 m, Δt = 1 day, C_0 = 10 kg/m^3, D = 10 m and V = 1 m/s.

The numerical solutions are compared with analytical solution at different times 5 days and 50 days in figure 3 using Δt = 1 day.

From case studies 1 and 2, it is obvious that the model is performing well as compared to the analytical solution. Hence, model may be applied to manage groundwater problems in probable real world situations.

CONCLUSIONS

A finite element based model has been formulated for groundwater pollutant transport. It consists of two modules, GWFM for groundwater flow and GWPTM for groundwater pollutant transport. The computer program for the model has been written in FORTRAN 77 and has been implemented on DEC AXE 3000 mainframe computer system. The results obtained for two case studies show that the model is working good and giving accurate results. As the model is general purpose, it can be used as a tool for solving any groundwater flow / pollution problem.

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