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A model of groundwater contaminant transport using the CVBEM

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Abstract. The Complex Variable Boundary Element Method or CVBEM has been used to develop a simple but powerful numerical analog of contaminant transport in a saturated, confined groundwater aquifer. The presented numerical technique is based upon a mean-square fit of the boundary conditions which includes the effects of sources and sinks defined within the problem domain. The numerical analogue produces locations of streamlines and the time-evolution of the contaminant front location.

1 Introduction

Potential flow theory may be used to depict streamlines of the groundwater flow for analyzing the extent of subsurface contaminant movement. With analytic functions, a two-dimensional flow field may be modeled by superposition of background flows, sources and sinks, and flows introduced by the boundary conditions. Thus, if the contaminant moves with the fluid in a steady groundwater flow, the application of analytic functions is of particular use in its transport study.

However, when time-dependent boundary conditions are present and dispersion-diffusion effects are significant, the steady state modeling approach becomes inappropriate. Another limitation of this technique is that it is not so suitable as to accommodate nonhomogeneity and anisotropy within the aquifer, because the complexity rapidly exceeds the modeling capability of the analytic function technique.

Due to the limitation of readily available analytic functions, many flow field problems are not easily solvable. The CVBEM, however, provides an immediate extension. That is, potential flow theory is utilized to solve analytically the groundwater flow field as provided by sources and sinks (groundwater wells and recharge wells), while the background flow conditions are modeled by means of a Cauchy integral collocated at nodal points specified along the problem boundary. The technique accommodates nonhomogeneity on a regional scale (i.e., homogeneous in large subdomains of the problem), and can include spatially distributed sources and sinks such as mathematically described by Poissons equation. Detail developments of the CVBEM numerical technique are given in Hromadka (1984a and b).

Both the boundary integral equation methods (BIEM) (Liggett and Liu 1983) and the complex variable boundary elements or CVBEM (Strack and Haitjema 1981a, 1981b, Hromadka 1984a, 1984b) are similar in that a boundary integral is solved by numerical integration resulting in a square, fully-populated matrix of an order equal to the number of nodes placed on the problem boundary. The presented numerical technique is based upon a mean-square fit of the boundary conditions which (1) includes the efforts of sources and sinks defined within the problem domain and (2) eliminates the need for a square matrix solution.

For steady state, two-dimensional, homogeneous-domain problems, the CVBEM develops an approximation function which combines an exact solution of the governing groundwater flow equation (Laplace equation) and approximate solutions of the boundary conditions. For unsteady flow problems, the CVBEM can be used to approximately solve the time advancement by implicit finite difference time-stepping analogous to domain models.

In this application, only the steady state two-dimensional flow problem will be considered in a homogeneous domain. In other words, application of the CVBEM contaminant transport model is restricted to steady state flow cases in which solute transport is by advection only. Due to the small coding requirements, the CVBEM program is operable on a typical 64K homecomputer.

2 Governing equations

For steady-state flow, the equation of continuity can be expressed as

$$\nabla \varrho V = 0, \tag{1}$$

where V is the velocity vector $V(u, v, w)$ and ϱ is the fluid density. If density variation is negligible, Eq. (1) reduces to

$$\nabla V = 0. \tag{2}$$

The velocity vector is related to the Darcys Law as follows:

$$V = -K_H \nabla \phi \tag{3}$$

in which $\nabla \phi$ is the gradient of total potential of head, having the dimension of energy per weight, or length. For a saturated system filled with a homogeneous fluid, ϕ includes only hydrostatic pressure potential (ϕ_p) and gravitational potential (G), i.e., $\phi = \phi_p + G$. In a more familiar hydraulics notation ϕ can be expressed as

$$\phi = \frac{p}{\gamma} + h \tag{4}$$

in which p is the hydrostatic pressure, γ denotes the specific weight of the fluids, and h signifies elevation in reference to an arbitrary datum. The hydraulic conductivity, K_H, is usually a function of several variables including the moisture volumetric content (ratio of fluid to total volume), porous media physical factors, and so forth.

Substituting the Darcy Eq. (3), into the continuity Eq. (2), one obtains

$$\nabla [K_H \nabla \phi] = 0. \tag{5}$$

If, in addition, K_H is constant, (for example, water of a constant viscosity in a homogeneous sand), Eq. (5) reduces to the Laplace equation.

$$\nabla^2 \phi = 0. \tag{6}$$

3 Use of complex variables

The use of the complex variables can facilitate the solution of a boundary value problem of the two-dimensional Laplace equation.

A complex variable function ω is related to the complex variable $z = x + iy$, by

$$\omega = f(z) = f(x + iy), \tag{7}$$

where ω may be separated into its real and imaginary parts

$$\omega = \phi(x, y) + i\psi(x, y) \tag{8}$$

in which ϕ and ψ are both real functions of x and y. For the function $\omega = f(z)$ to be analytic, the necessary and sufficient conditions are that ϕ and ψ be single-valued and that they satisfy the Cauchy-Riemann equations, i.e.,

$$\frac{\partial\phi}{\partial x}=\frac{\partial\psi}{\partial y}, \quad \frac{\partial\phi}{\partial y}=-\frac{\partial\psi}{\partial x}. \tag{9}$$

The lines defined by $\phi=(x,y)=$const are called equipotential (or potential) lines. The lines defined by $\psi=\psi(x,y)=$const are streamlines. Finding gradients for these two families of curves and using the Cauchy-Riemann Eqs. (9), it can be shown that the equipotential lines and the streamlines are orthogonal.

4 Flow field model

Due to the linearity of Laplaces equation, one can superimpose as many flow components as required to obtain the general expression for the complex velocity potential of the entire system. A potential function $F(z)$ which described one or several point sources of contaminant recharge, together with some groundwater discharging wells, combined with a uniform regional groundwater flow regime, is developed that exactly satisfies the Laplace equation in domain Ω by

$$F(z)=\hat{\omega}(z)+\sum_{i=1}^{n}\frac{Q_i}{2\pi T}\ln(z-z_i) \quad z\in\Omega, \tag{10}$$

where Q_i is the discharge from well i (of n) located at z_i [i.e. (+) for a sink, (−) for a source], T is the transmissivity of a confined aquifer, and $\hat{\omega}(z)$ is a CVBEM approximator representing the background flow field. In Eq. (10), $F(z)$ must satisfy the boundary conditions

$$\xi(z)=\delta\phi(z)+i(1-\delta)\psi(z) \quad z\in\Gamma, \tag{11}$$

where $\delta=1$ if $\phi(z)$ is known, $\delta=0$ if $\psi(z)$ is known, and $\xi(z)$ is a boundary-condition distribution along Γ.

The source and sink terms included in Eq. (10) represent an exact model for steady state flow. Thus, $\xi(z)$ must be modified in order to develop a CVBEM $\hat{\omega}(z)$ by

$$\xi^*(z)=\xi(z)-\sum_{i=1}^{n}\frac{Q_i}{2\pi T}\ln(z-z_i) \quad z\in\Gamma. \tag{12}$$

The flow field is then determined by collocating $\hat{\omega}(z)$ at each node $z_j\in\Gamma$ according to the boundary-condition distribution of $\xi^*(z)$. The resulting analytic function $F(z)$ describes the CVBEM model. In Eq. (12), $\xi^*(z)$ is defined according to the real and imaginary parts as given in Eq. (11).

5 Poisson equation

Given a continuous distribution of sources (such as from precipitation) in a flow field in domain Ω, the steady state flow model must be extended to accommodate the Poisson equation, with k as a constant.

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=k. \tag{13}$$

Equation (13) can be modeled by choosing a particular solution ϕ_p such that

$$\frac{\partial^2\phi_p}{\partial x^2}+\frac{\partial^2\phi_p}{\partial y^2}=k. \tag{14}$$

For example, $\phi_p=k(x^2+y^2)/4$ is a suitable choice (an infinity of other particular solutions are available). After choosing ϕ_p, the boundary condition function $\xi(z)$ is modified in order to develop

$\hat{\omega}(z)$ by

$$\xi^*(z)=\xi(z)-\sum_{i=1}^{n}\frac{Q_i}{2\pi T}\ln(z-z_i)-\phi_p(z) \quad z\in\Gamma. \tag{15}$$

The CVBEM approximator $\hat{\omega}(z)$ is collocated at nodes z_j with respect to the $\xi^*(z)$ function. Thus, the Poisson equation is exactly solved by

$$F(z)=\hat{\omega}(z)+\sum_{i=1}^{n}\frac{Q_i}{2\pi T}\ln(z-z_i)+\phi_p(z). \tag{16}$$

The above procedure can be extended to the relation

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=f(x,y) \tag{17}$$

by choosing a ϕ_p such that (17) is satisfied, and proceeding with the development of an appropriate CVBEM $\hat{\omega}(z)$ in the same way.

6 Solute transport model

The solute transport mechanism is assumed only applicable to the modeling of steady state, advective contaminants, for those which move with the groundwater flow. The solute-transport process is approximated by calculating point-flow velocities given by the derivative of the potential function $\phi(z)$ where

$$\phi(z)=\operatorname{Re}F(z). \tag{18}$$

The extent or boundary of the subsurface contamination is then evaluated according to point values of the flow velocity and the time increment selected. Point flow velocities are estimated as

$$u=-K\frac{\partial\phi}{\partial x}/\theta_0, \tag{19a}$$

$$v=-K\frac{\partial\phi}{\partial y}/\theta_0, \tag{19b}$$

where (u,v) are (x,y)-direction soil-water flow velocities, K is the saturated hydraulic conductivity, and θ_0 is the effective porosity of the aquifer material (a retardation factor r can be included in the denominator of Eq. (19) in order to account for contaminant transport velocities being less than the actual field velocity or specific discharge).

The velocity of a contaminant particle is used to estimate the distance traveled along a flow field streamline by the approximations

$$\frac{dx^*}{dt}=u, \tag{20a}$$

$$\frac{dy^*}{dt}=v, \tag{20b}$$

where in the above (x^*,y^*) are the coordinates of the subject contaminant particle.

7 The CVBEM (using the L^2 norm)

The CVBEM approximation function for linear (straight-line interpolation) basis functions results in the complex function (Hromadka 1984a, 1984b)

$$\hat{\omega}(z)=\sum_{j=1}^{m}c_j(z-z_j)\ln(z-z_j), \tag{21}$$

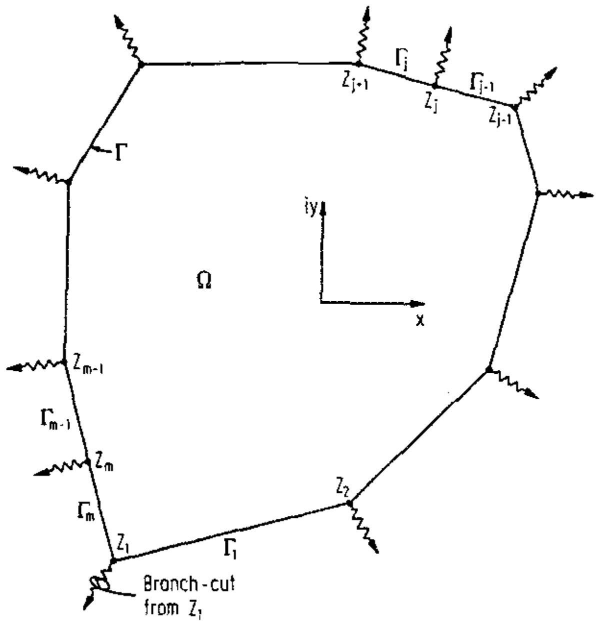

Fig. 1. The analytic continuation of $\hat{\omega}(z)$ to the exterior of $\Omega \cup \Gamma$. Note: Branch cuts along Γ at nodes z_j

where the c_j are complex constants $c_j = a_j + \mathrm{i}b_j$, z_j are nodal points $(j = 1, 2, \ldots, m)$ defined on the problem boundary Γ (simple closed contour) and $\ln(z - z_j)$ is the principal value complex logarithm function with branch cuts specified to intersect Γ only at z_j (Fig. 1). Then $\hat{\omega}(z)$ is analytic over $\Omega \cup \Gamma \setminus \{z_j\}$ and uniformly continuous over $\Omega \cup \Gamma$. Here, Ω is a simply connected domain enclosed by Γ. In fact, $\hat{\omega}(z)$ is analytic over the entire complex plane less the branch cuts. The c_j are calculated in the CVBEM technique by collocating to the boundary condition values known at the nodal points [Hromadka (1984)].

The c_j are calculated in the L^2 norm sense by finding the best choice of c_j to minimize the mean-square error in matching the boundary condition values continuously along Γ. Notation is used for the known and unknown function values along Γ.

$$\begin{aligned} \omega(\zeta) &= \Delta\xi_k(\zeta) + \Delta\xi_u(\zeta) \\ \hat{\omega}(\zeta) &= \Delta\hat{\xi}_k(\zeta) + \Delta\hat{\xi}_u(\zeta) \end{aligned} \quad \zeta \in \Gamma, \tag{22}$$

where $\omega(z)$ is the solution to the boundary value problem over $\Omega \cup \Gamma$, $\hat{\omega}(z)$ is the CVBEM approximation over $\Omega \cup \Gamma$, Δ is a descriptor function such that $\Delta = 1, \mathrm{i}$ depending whether the associated ξ_x or $\hat{\xi}_x$ function is the real or imaginary term and ζ is the notation for the case $z \in \Gamma$. Then the objective is to compute the c_j which, for a given nodal distribution on Γ, minimize

$$I = \|\xi_k - \hat{\xi}_k\|_2^2 = \int_\Gamma (\xi_k - \hat{\xi}_k)^2 \, \mathrm{d}\Gamma. \tag{23}$$

8 Orthogonal CVBEM functions and the best approximation

The CVBEM approximation function of (21) can be written as

$$\hat{\omega}(z) = \sum_{j=1}^{m} c_j f_j, \tag{24}$$

where $f_j = (z - z_j)\ln(z - z_j)$. The Gram-Schmidt procedure can be used to orthogonalize the f_j such that

$$\hat{\omega}(z) = \sum_{j=1}^{m} \gamma_j g_j, \tag{25}$$

where γ_j are complex constants and

$$(g_j, g_k) = \int_{\Gamma} g_j g_k \mathrm{d}\Gamma = \begin{cases} 1, & j=k \\ 0, & j \neq k \end{cases}. \tag{26}$$

In (26), (g_j, g_k) is the notation for the inner product.

The boundary conditions on Γ are given by ξ_k where $\phi(\zeta)$ is known continuously on the contour Γ_ϕ and $\psi(\zeta)$ is known continuously on Γ_ψ where $\Gamma_\phi + \Gamma_\psi = \Gamma$ and $\Gamma_\phi \cap \Gamma_\psi$ only at nodal points. The Γ_ϕ and Γ_ψ can be composed of a finite number of contours. Then the γ_j are computed which minimize

$$I = \int_{\Gamma_\phi} (\phi(\zeta) - \mathrm{Re}\, \Sigma \gamma_j g_j) \mathrm{d}\Gamma + \int_{\Gamma_\psi} (\psi(\zeta) - \mathrm{Im}\, \Sigma \gamma_j g_j) \mathrm{d}\Gamma. \tag{27}$$

Because the g_j are orthogonal, the γ_j are directly computed by

$$\gamma_j = (\xi_k, g_j)/(g_j, g_j). \tag{28}$$

Then the best approximation (in the L_2-norm) is given by

$$\hat{\omega}(z) = \sum_{j=1}^{m} (\xi_k, g_j) g_j / (g_j, g_j). \tag{29}$$

The c_j are then computed by back-substitution of the $\gamma_j g_j$ functions into the $c_j f_j$ functions. It is noted that by this approach, the c_j are computed directly without the use of a matrix system generation or matrix solution. This is important due to boundary integral methods resulting in the solution of fully populated, square matrix systems.

9 Orthogonal vector systems and the best approximation

Let F_j be linearly independent vectors of dimension n, for $j = 1, 2, \ldots, m$. Then the Gram-Schmidt procedure can be used to construct orthogonal vectors $\mathbf{G}_j$ of dimension n such that the dot product gives

$$G_j G_k = \begin{cases} 1, & j=k \\ 0, & j \neq k \end{cases}. \tag{30}$$

Let B be a vector of dimension n. Then the best approximation of B in the subspace spanned by the G_j is given by the vector A where

$$A = \sum_{j=1}^{m} \eta_j G_j \tag{31}$$

with

$$\eta_j = (B G_j)/(G_j G_j). \tag{32}$$

The corresponding approximation to B with respect to the original F_j vectors is

$$A = \sum_{j=1}^{m} C_j F_j, \tag{33}$$

where the C_j are computed by back-substitution of $\eta_j G_j$ into the respective F_j components.

10 Representation of the CVBEM approximation function by a dimension *mn* vector space

Let Γ be discretized into m boundary elements Γ_j, $j = 1, 2, \ldots, m$. On each element, define n interior evaluation points (usually evenly spaced), resulting in a total of mn points t_i on Γ. For each function f_j (see (24)), develop the vector F_j of dimension mn by

$$F_j = \{ f_j(t_i); \quad i = 1, 2, \ldots, mn \}. \tag{34}$$

In (34), the coordinates of t_i are consistent for each vector F_j, $j = 1, 2, \ldots, m$, such that points

$(t_1, t_2, \ldots, t_n)$ occur in boundary element Γ_1. The resulting vectors $\boldsymbol{F}_j$ form the basis of a subspace F_{mn} where each vector $\boldsymbol{F} \in \boldsymbol{F}_{mn}$ is given by

$$\boldsymbol{F} = \sum_{j=1}^{m} \eta_j \boldsymbol{F}_j. \tag{35}$$

Similarly the boundary condition values defined on Γ can be represented by the vector $\boldsymbol{B}$ where

$$\boldsymbol{B} = \{\xi_k(t_i);\quad i = 1, 2, \ldots, mn\}. \tag{36}$$

The best approximation of the vector $\boldsymbol{B}$ (in the l_2-norm analogy of the L_2-norm) by a vector $\boldsymbol{A} \in \boldsymbol{F}_{mn}$ is given directly by (31) and (32). The corresponding estimate of the best approximation $\hat{\omega}(z)$ is given by

$$\hat{\omega}(z) = \sum_{j=1}^{m} \eta_j g_j. \tag{37}$$

Thus in the above, the best approximation for $\hat{\omega}(z)$ is estimated by using the best approximation from a vector space spanned by the vectors $\boldsymbol{G}_j$.

11 Implementation

A FORTRAN computer program was prepared which developed the best approximation in a vector space (of dimension mn) in order to estimate the c_j coefficients of Eq. (21). The basic steps used in the program are as follows:

1. Data entry of nodal point (m) coordinates and boundary values.
2. Number of evaluation points entered (n).
3. Develop dimension mn vectors $\boldsymbol{F}_j, j = 1, 2, \ldots, m$.
4. Develop dimension mn vector $\boldsymbol{B}$ of boundary values.
5. Develop orthogonal vectors $\boldsymbol{G}_j, j = 1, 2, \ldots, m$.
6. Compute vector coefficients η_j.
7. Back substitute $\boldsymbol{G}_j$ vectors into $\boldsymbol{F}_j$ vectors and compute the coefficients $C_j; j = 1, 2, \ldots, m$.
8. Define $c_j = C_j$ to determine the CVBEM approximation function, $\hat{\omega}(z)$.

It is noted that $c_j = \alpha_j + i\beta_j$. Thus the above program steps involve two vectors for each C_j.
That is from (21),

$$\hat{\omega}(z) = \sum_{j=1}^{m} \alpha_j[(z - z_j)\ln(z - z_j)] + \sum_{j=1}^{m} \beta_j[i(z - z_j)\ln(z - z_j)]. \tag{38}$$

Hence the f_j corresponding to the c_j have two separate components which are used, respectively, with the α_j and β_j. Consequently, for m nodes there are $2m$ coefficients to be computed.

12 Applications of CVBEM program

Application 1: Fig. 2 shows a completely penetrating groundwater well (discharge 50 m^3/hr) located at the coordinates (300, 300) in a homogeneous isotropic aquifer of thickness 10 m. Contaminated water is being recharged (recharge of 50 m^3/hr) at a second well (injection well) located at the coordinates (300, −300) with a distance of 848.5 m from the supply well (discharge well). Effective porosity is 0.25, saturated hydraulic conductivity is 1 m/hr, and negligible background groundwater flow is assumed. Retardation is assumed to be 1.

Depicted in Fig. 2 are the limits of groundwater contamination corresponding to model times of 0.5, 2 and 4 years. Additionally, the CVBEM model predicts a first arrival of contamination of time 4.33 years for injected water to reach the pumping site which agrees well with the estimate by Javendal et al. (1985) of 4.3 years.

Application 2: An additional discharge well is added at the coordinate (500, 500) in application 1. Fig. 3 depicts the contaminant front at 0.5, 2 and 4 years. Because the upper discharge well is slightly closer to the injection well, it takes 4.22 years and 4.61 years for the contaminant water to reach the upper and lower discharge wells, respectively.

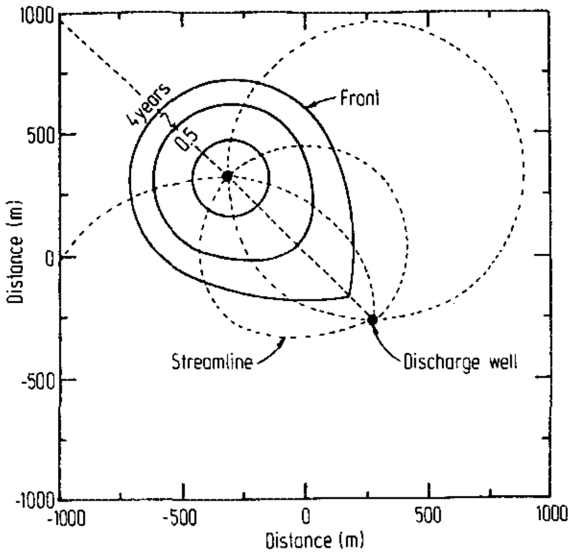

Fig. 2

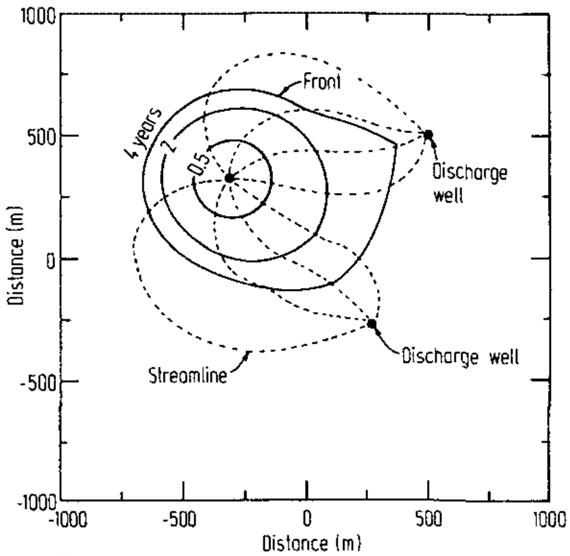

Fig. 3

Figs. 2 and 3. Flowline pattern and front positions between injection 2 and production well for application 1; 3 and two production wells for application 2

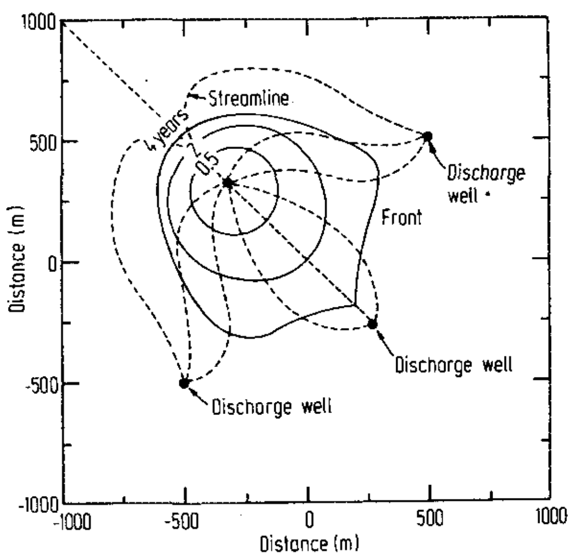

Fig. 4

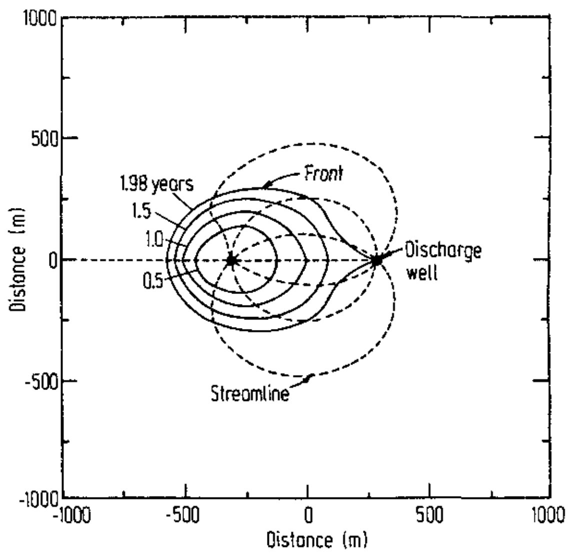

Fig. 5

Figs. 4 and 5. Flowline pattern and front positions between injection 4 and three production wells for application 3; 5 and productions wells for application 4

Application 3: Third discharge well is added at the coordinate (−500, −500) in application 2. Figure 4 depicts the contaminant front at 0.5, 2 and 4 years. It takes 4.32 years for the contaminant water to reach the middle discharge well (−300, 300) and about 5.58 years for the contaminant water to reach the other two production wells.

Application 4: In this problem, the injection well and the discharge well are located at (−300,0) and (300,0), respectively. A differential potential of 2 m is assumed across the western and eastern boundaries. The potential along the northern and southern boundaries are assumed to be linearly distributed. Fig. 5 depicts the contaminant front at 0.5, 1, 1.5 and 1.98 years. The contaminant water takes about 2 years to reach the discharge well.

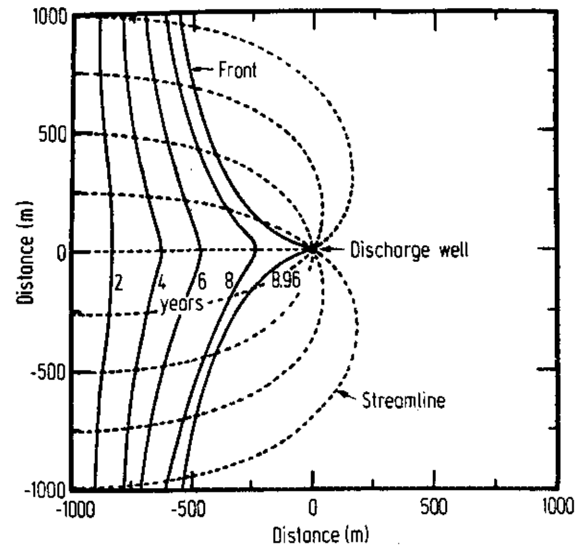

Fig. 6

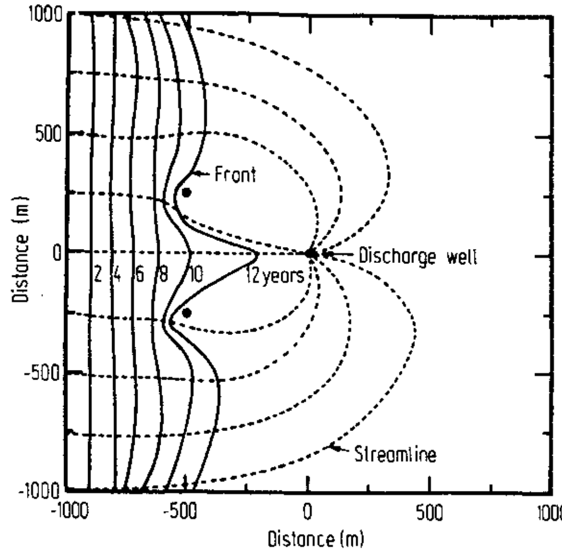

Fig. 7

Figs. 6 and 7. Flowline pattern and front positions between 6 equipotential boundary and discharge well; 7 two retarding wells and production well for application 5

Application 5: Let's consider the steady flow pattern produced by a single pumping well whose strength equals to 50 m^3/hr at (0,0) near a landfill site with an equipotential boundary $\phi = 2$ m along $x = -1000$. It took the contaminant front 8.96 years to reach the pumping well. Two additional injection wells were installed at $(-500, 250)$ and $(-500, -250)$ with strength equal to 10 m^3/hr, to retard the contaminant front. Fig. 6 and 7 depict the front movements of these two case problems.

12 Conclusions

In this paper, the CVBEM is reanalyzed to eliminate the need for a square matrix solution. The new method is based on generalized Fourier series theory, and it satisfies the boundary conditions in a least-square (L^2) sense. The resulting model is identical in capability as the previous CVBEM model [Hromadka (1984b)], but provides the significant improvements of 1. satisfying boundary conditions in a L^2-norm, and 2. eliminates the matrix generation requirements.

The new CVBEM has been used to develop a numerical analogue of background potential flow in the domain where sources and sinks are defined. The program develops flow-fields and the time evolution of the flow-field motion for contaminant transport. Although this study focuses upon groundwater flow problems, the numerical analogue can be extended to other equivalent problems such as involved in heat and mass transport in homogeneous domains.

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