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Complex Variable Boundary Element Solution of Groundwater Contaminant Transport

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ABSTRACT

The estimation of the location and propagation of a plume in a groundwater basin is an important problem in contaminant transport engineering. Typically, finite element models are used to develop solutions as to the location and movement of the plume in the basin. In this paper, the Complex Variable Boundary Element Method or CVBEM is used to develop streamlines and plume shape of the moving contaminant. Arrival times of the contaminant at pumping wells can be estimated, and the choice for the location of injection wells analyzed by use of this method. The CVBEM program is user-interactive, and can be operated on IBM compatible personal computers.

INTRODUCTION

Potential flow theory may be used to depict streamlines of the groundwater flow for analyzing the extent of subsurface contaminant movement. Especially in the preliminary study, the potential flow theory can be used to determine whether or not a more sophisticated study based on a long period of observation and expensive data collection is required.

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 anistropy 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 Poisson's equation. Detail developments of the CVBEM numerical technique are given in Hromadka[1,2] and Hromadka and Yen [3,4].

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.

Governing Equations

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

$$\vec{\nabla} \cdot \rho \vec{V} = 0 \tag{1}$$

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

$$\vec{\nabla} \cdot \vec{V} = 0 \tag{2}$$

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

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

in which $\vec{\nabla}\phi$ is the gradient of total potential of head, having the dimension of energy per weight, or length. Substituting the Darcy equation, (3), into the continuity equation, (2), one obtains

$$\vec{\nabla} \cdot [K_H \vec{\nabla} \phi] = 0 \tag{4}$$

If, in addition, K_H is constant, (for example, water of a constant viscosity in a homogeneous sand), Eq. (4) reduces to the Laplace equation

$$\nabla^2\phi = 0 \tag{5}$$

The CVBEM continues by using (8) to develop m equations as a function of the m unknowns associated with the undetermined nodal values of either $\bar{\phi}$ or $\bar{\psi}$ at each node. That is, $\bar{\omega} = \bar{\phi} + i\bar{\psi}$ where $\bar{\phi}$ and $\bar{\psi}$ are nodal values of the potential and stream functions respectively.

Flow Field Model

Due to the linearity of Laplace's 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 of 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

$$F(z) = \hat{\omega}(z) + \sum_{i=1}^{n} \frac{Q_i}{2\pi T} \operatorname{Ln}(z - z_i), \; z \in \Omega \qquad (6)$$

which 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. (6), F(z) must satisfy the boundary conditions

$$\xi(z) = \delta\phi(z) + i(1-\delta)\,\psi(z), \; z \in \Gamma \qquad (7)$$

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. (6) represent an exact model for steady state flow. Thus, $\xi(z)$ must be modified in order to develop a CVBEM $\hat{\omega}(z)$ by

$$\xi^*(z) = \xi(z) - \sum_{j=1}^{n} \frac{Q_i}{2\pi T} \operatorname{Ln}(z - z_i), \; z \in \Gamma \qquad (8)$$

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. (8), $\xi^*(z)$ is defined according to the real and imaginary parts as given in Eq. (7).

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.

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = k \qquad (9)$$

Equation (9) can be modeled by choosing a particular solution ϕ_p such that

$$\frac{\partial^2 \phi_p}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = k \qquad (10)$$

For example, $\phi_p = \frac{k}{4}(x^2 + y^2)$ 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

$$\xi^*(z) = \xi(z) - \sum_{i=1}^{n} \frac{Q_i}{2\pi T} \mathrm{Ln}\,(z - z_i) - \phi_p(z),\ z \in \Gamma \qquad (11)$$

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

$$F(z) = \hat{\omega}(z) + \sum_{i=1}^{n} \frac{Q_i}{2\pi T} \mathrm{Ln}\,(z - z_i) + \phi_p(z) \qquad (12)$$

The above procedure can be extended to the relation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f(x,y) \qquad (13)$$

by choosing a ϕ_p such that Eq. (13) is satisfied, and proceeding with the development of an appropriate CVBEM $\hat{\omega}(z)$ in the same way.

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

$$\phi(z) = \mathrm{Re}\ F(z) \qquad (14)$$

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

$$u = -K \frac{\partial \phi}{\partial x} / \theta_0 \qquad (15a)$$

$$v = -K \frac{\partial \phi}{\partial y} / \theta_0 \qquad (15b)$$

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 material. (A retardation factor, r, can be included in the denominator of Eq. (15) 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

$$\frac{dx^*}{dt} = u \qquad (16a)$$

$$\frac{dy^*}{dt} = v \qquad (16b)$$

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

<u>CVBEM (Using the Collocation Method)</u>

The CVBEM has been shown to be a powerful numerical technique for the approixmation of properly posed boundary-value problems involving the Laplace equation (Hromadka[2]). The keystone of the numerical approach is the integral function

$$\hat{\omega}(z) = \frac{1}{2\pi i} \int_{\Gamma} \frac{G(\zeta)d\zeta}{\zeta - z} \qquad (17)$$

where Γ is a simple closed contour enclosing a simply connected domain Ω; ζ is the variable of integration with $\zeta \in \Gamma$; z is a point in Ω; and the direction of integration is in the usual counterclockwise (positive) sense (fig. 1). The function $G(\zeta)$ is a global trial function which is continuous on Γ. The linear global trial function is defined by

$$G(\zeta) = \sum_{j=1}^{m} \delta_j \left(N_j \bar{\omega}_j + N_{j+1} \bar{\omega}_{j+1}\right) \qquad (18)$$

where $\delta_j = 1$ if $\zeta \in \Gamma_j$, and $\delta_j = 0$ if $\zeta \notin \Gamma_j$. In this case, the functions N_j and N_{j+1} are the usual linear basis functions. From the definition of $G(\zeta)$ we have

$$\int_{\Gamma} \frac{G(\zeta)d\zeta}{\zeta - z} = \int_{U\Gamma_j} \frac{G(\zeta)d\zeta}{\zeta - z} = \sum_{j=1}^{m} \int_{\Gamma_j} \frac{G(\zeta)d\zeta}{\zeta - z} = \sum_{j=1}^{m} \int_{\Gamma_j} \frac{(N_j \bar{\omega}_j + N_{j+1} \bar{\omega}_{j+1})d\zeta}{\zeta - z} \qquad (19)$$

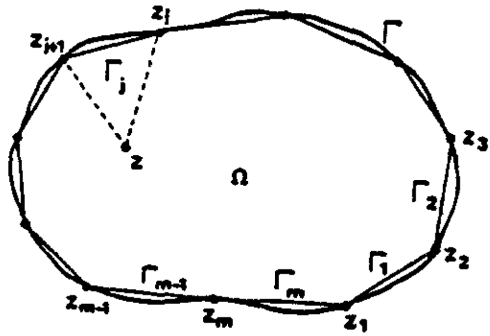

Figure 1. CVBEM Boundary Discretization

Γ_j = Boundary element linking nodes j and j+1;
z_j = Nodal coordinate for node j, $(z_{m+1} = z_1)$;
Γ = Natural boundary

The CVBEM approximation function for linear (straight-line interpolation) basis functions results in the complex function

$$\hat{\omega}(z) = \sum_{j=1}^{m} c_j(z - z_j) \, \mathrm{Ln}\,(z - z_j) \tag{20}$$

where the c_j are complex constants $c_j = a_j + ib_j$; z_j are nodal points $(j = 1,2,\cdots,m)$ defined on the problem boundary Γ (simple closed contour); and $\mathrm{Ln}(z - z_j)$ is the principal value complex logarithm function with branch cuts specified to intersect Γ only at z_j (see Fig. 2). Given m nodes specified on Γ_j, we necessarily know either $\bar{\Phi}$ or $\bar{\Psi}$ (not both) at each z_j, $j = 1,2,\cdots,m$. Then to estimate the remaining m nodal values, $\hat{\omega}(z)$ is collocated in the form of a Fredholm equation which resulting in the solution of fully populated, square matrix system.

CVBEM (Using the L_2 Norm)

The CVBEM model is now expanded as a generalized Fourier series--eliminating the matrix solution entirely. 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.

$$\left.\begin{aligned} \omega(\zeta) &= \Delta\xi_k(\zeta) + \Delta\xi_u(\zeta) \\ \hat{\omega}(\zeta) &= \Delta\hat{\xi}_k(\zeta) + \Delta\hat{\xi}_u(\zeta) \end{aligned}\right\} \quad \zeta \in \Gamma \tag{21}$$

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 $\Delta = 1,i$ depending whether the

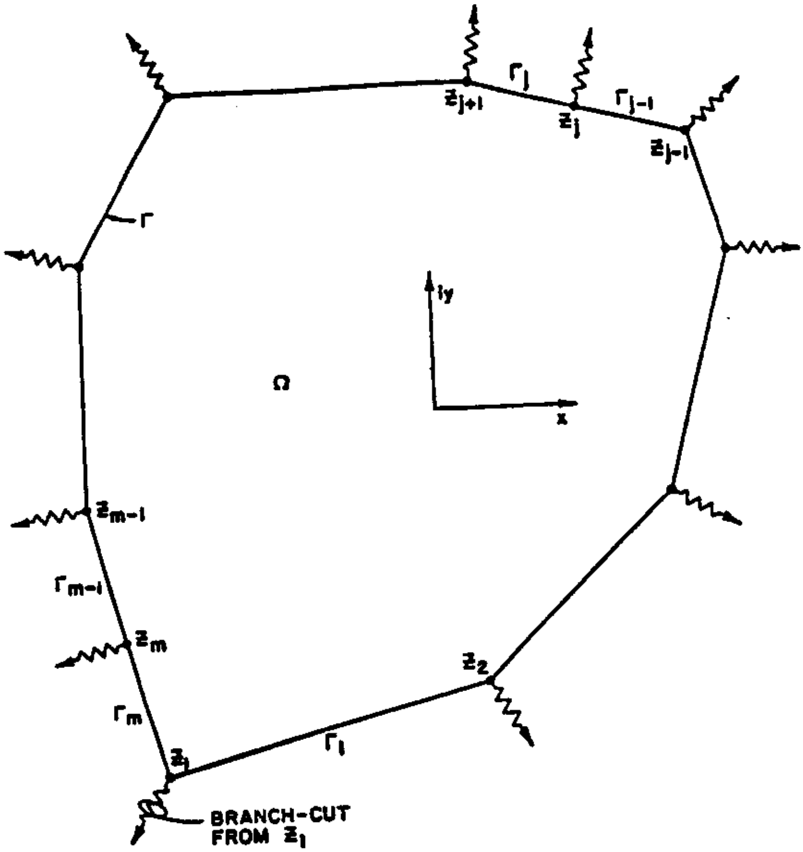

Figure 2. The Analytic Continuation of $\hat{\omega}(z)$ to the Exterior of $\Omega \cup \Gamma$

Note: Branch Cuts along Γ at Nodes z_j

associated ξ_x or $\hat{\xi}_x$ function is the real or imaginary term; and ζ is notation for the case of $z \varepsilon \Gamma$. Then the objective is to computer the c_j which, for a given nodal distribution on Γ, minimize

$$I = ||\xi_k - \hat{\xi}_k||_2^2 = \int_\Gamma (\xi_k - \hat{\xi}_k)^2 \, d\Gamma \tag{22}$$

The CVBEM approximation function of (20) can be written as

$$\hat{\omega}(z) = \sum_{j=1}^{m} c_j f_j \tag{23}$$

where $f_j = (z - z_j)\,\mathrm{Ln}\,(z - z_j)$. The Gram-Schmidt procedure can be used to orthogonalize the f_j such that

$$\hat{\omega}(z) = \sum_{j=1}^{m} \gamma_j g_j \tag{24}$$

where γ_j are complex constants and

$$(g_j, g_k) = \int_{\Gamma} g_j g_k \, d\Gamma = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases} \tag{25}$$

In (25), (g_j, g_k) is notation for the inner product.

The boundary conditions on Γ are given by ξ_k where $\phi(\zeta)$ is known continuously on 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

$$I = \int_{\Gamma_\phi} (\phi(\zeta) - \mathrm{Re}\, \Sigma\gamma_j g_j) d\Gamma + \int_{\Gamma_\psi} (\psi(\zeta) - \mathrm{Im}\, \Sigma\gamma_j g_j) d\Gamma \tag{26}$$

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

$$\gamma_j = (\xi_k, g_j)/(g_j, g_j) \tag{27}$$

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

$$\hat{\omega}(z) = \sum_{j=1}^{m} (\xi_k, g_j) g_j/(g_j, g_j) \tag{28}$$

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.

Both models show compatible results for the following groundwater contaminant problems.

<u>Application 1</u>. Figure 3 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 discharged (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. 3 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 Javendal et al.[5] estimate of 4.3 years.

Application 2. Two discharge wells are added at the coordinates (+500, +500) in application 1. Figure 3 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.

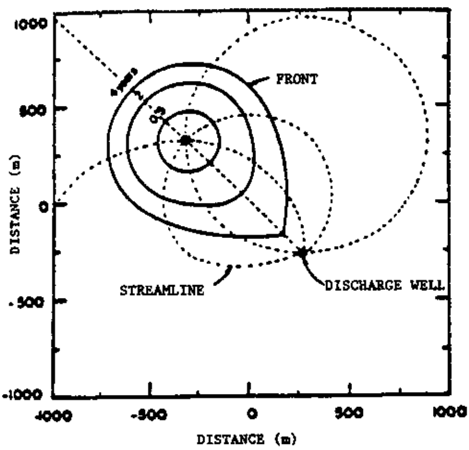

Fig. 3. Flowline pattern and front positions between injection and production well for application 1

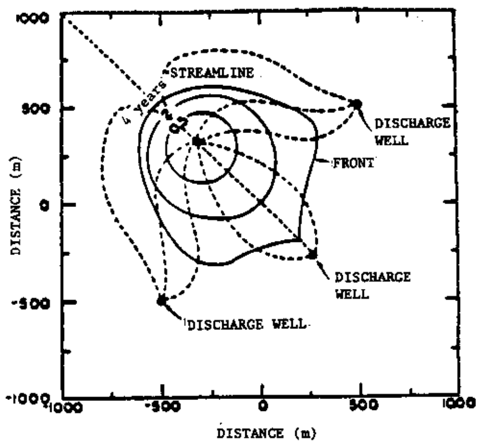

Fig. 4. Flowline pattern and front positions between injection and three production wells for application 2

Application 3. Let's consider the steady flow pattern producted 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. Figures 5 and 6 depict the front movements of these two case problems.

Application 4. In this problem, a liquid-waste disposal pond with a diameter of 100 m fully penetrates the aquifer is added to application 3. The center of this pond has coordinates of

(500, 500) on the Cartesian system shown in Fig. 7. Liquid level in the pond is such that the volume rate of leachate leaving the pond is about 20 m^3/hr. It takes 15.7 years and 7.3 years for the contaminant liquid to reach the discharge well from the left boundary and from the disposal pond, respectively.

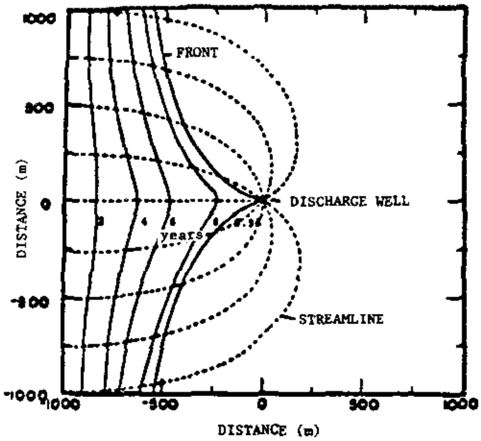

Fig. 5. Flowline pattern and front positions between equipotential boundary and discharge well

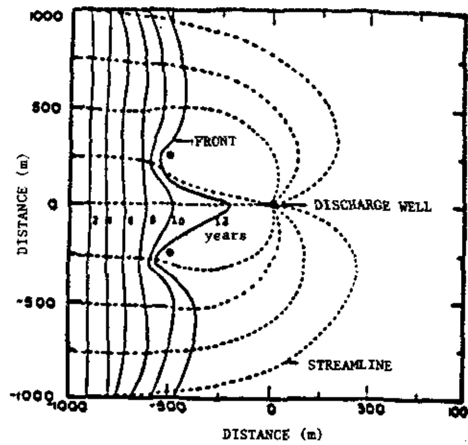

Fig. 6. Flowline pattern and front positions between retarding wells and production well for application 3

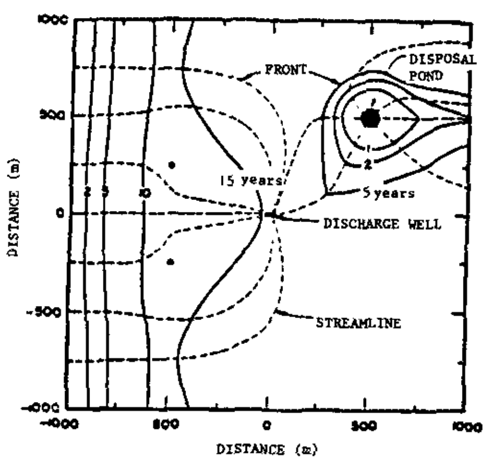

Fig. 7. Flowline pattern and front positions for application 4

Summary and Conclusions

In this paper, the CVBEM collocation and L_2 norm methods are used to develop models of steady-state, advective, contaminant transport in ground-water. Because with the CVBEM approach the Laplace and Poisson partial differential equations are solved exactly, all modeling error occurs in matching the prescribed boundary conditions.

For the same nodal displacement, on the domain boundary both models show compatible results in matching the boundary conditions. It has been found that less nodal points and execution time for the collocation method achieved the same accuracy of stream and potential functions than the L_2 model that used more nodal points and execution time. Therefore, a collocation method is recommended for the regional goundwater contaminant problem.

Because the modeling technique is based upon a boundary integral equation approach, domain mesh generators or control-volume (finite element) discretizations are not required. Nodal points are required only along the problem boundary rather than in the interior of the domain.

Consequently, the computer-coding requirements are small and can be accommodated by many currently available home computers that supports a FORTRAN compiler. Although this study focuses upon groundwater flow problems, the numerical analog can be extended to other equivalent problems such as involved in heat and mass transport in homogeneous domains.

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