Modeling steady-state, advective contaminant transport by the complex variable boundary element method

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A model of two-dimensional, steady-state, advective subsurface contaminant transport in ground-water is developed based on the CVBEM (complex variable boundary element method). The CVBEM model includes an exact solution of the governing partial differential flow equations classified as Laplacian or Poisson. The model includes point sources and sinks, distributed sources and sinks, and the accommodation conditions specified on the problem boundary. Because the numerical technique is a boundary integral equation method, the computer requirements are small and can be accommodated by many currently available microcomputers.

Key Words: complex variable boundary element method, solute transport, approximate boundary

INTRODUCTION

Mathematical modeling techniques which have been developed for use in predicting the extent of subsurface contamination of ground water, in general order of complexity, fall into three broad categories: (1) analytical techniques; (2) quasi-analytical techniques; and (3) numerical modeling techniques based on domain methods such as finite difference, integrated finite difference, or finite element.

Each of the modeling categories develops a mathematical statement which satisfies the flow continuity and mass balance equations. However, as the problem requirements and conditions increase in complexity, the minimum level of sophistication needed to model the problem generally passes between the modeling categories.

For simple time-dependent solute transport within a domain including steady and uniform ground-water flow, analytical solutions are available for several one-dimensional or radial flow regimes. For example, Van Genuchten and Alves[1] summarize the mathematical solutions to several one-dimensional convective-dispersive solute transport problems. Generally, such mathematical solutions are based on limited ground-water flow conditions such as uniform flow. Additionally, the assigned contaminant source mechanism often limits the modeling application to highly idealized situations. However, for studies which afford little data for identification of the various flow parameters, the analytical solution technique can be used to provide preliminary estimates as to the time scale and the potential extent of the contamination.

The second category of modeling techniques utilizes well-known potential flow theory to develop streamlines of the underlying ground-water flow (that is, the Laplace equation). Using analytic functions of the complex variable, a two-dimensional flow field is modeled by superposition of flow patterns, sources and sinks, and boundary flow conditions.

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For the type of flow problems where the ground-water flow field is steady-state and the contaminant transport moves with the fluid, the quasi-analytical approach provides a powerful tool for study purposes. However, for cases where time-dependent boundary conditions and dispersion-diffusion effects are significant, the needed minimum modeling sophistication transcends to the third category.

Another major limitation of the quasi-analytic technique is the accommodation of nonhomogeneity and anisotropy within the aquifer, and the capability to model the underlying flow field as a function of the boundary conditions rather than as a prescribed potential flow field.

The third category of modeling techniques is based on the well-known domain numerical methods of finite difference, integrated finite difference, or finite element. Using such a model approach requires the discretization of the domain into control volumes or finite elements. Each element has an associated parameter set which accommodates for the nonhomogeneity of the aquifer, fluid properties, and contaminant properties. Flow conditions and desired contaminant transport mechanisms can then be modeled by the incorporation of various flow subprograms or bookkeeping algorithms which simulate particular transport processes.

Associated with numerical methods is the complications of calibrating the model to meet known physical conditions, and the potential for numerical error in satisfying the governing flow equations and the specified boundary conditions. For example, the analytical and quasi-analytical techniques exactly satisfy the governing flow equations; in comparison, the domain numerical methods only satisfy the governing steady-state flow equations for basic scenarios such as uniform flow. In use of numerical methods with more complex flow situations, attention is required as to numerical stability, choice of discretization, timestep advancement and timestep size, and the overall accuracy of the coupled numerical models.

Various domain numerical models are available which include submodels for accommodating particular transport

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processes. A detailed tabulation of 32 such domain models is given in Javendal and others,[2] which itemizes the numerical modeling approaches and ancillary submodels, and includes transport processes.

A new direction for subsurface contaminant transport modeling is the use of the complex variable boundary element method or CVBEM.[3] This modeling technique simulates two-dimensional contaminant transport as an extension of the quasi-analytical approach. That is, potential flow theory is utilized to develop the underlying groundwater flow field as provided by sources and sinks (groundwater wells and recharge wells), but 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. An early application of the Cauchy integral for solving groundwater flow problems is contained in Hunt and Isaacs.[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 paper, only the steady-state two-dimensional flow problem will be considered in a homogeneous domain. The extension to unsteady flows or nonhomogeneous domains is referenced to Hromadka[3] or Brebbia.[5] Other real variable boundary element models are discussed in Liggett,[6] and in Liu and Liggett.[7,8] A new development in this paper will be the solution of the Poisson equation in a homogeneous domain; this represents the first time that the CVBEM has been applied to this class of partial differential equations.

Application of of the CVBEM contaminant transport model in this paper is restricted to steady-state flow cases in which solute transport is by advection only. That is, mass transport by diffusion and dispersion is not included. However, it is noted that the CVBEM model requires only a limited quantity of data, and does not require the discretization of the domain into a mesh or set of control volumes of finite elements. Additionally, because of the small number of nodal points required, the computer program can be accommodated on most currently available microcomputers with a FORTRAN capability.

Modeling error evaluation is readily available by use of an approximate boundary approach. Because the CVBEM model provides an exact solution to the partial differential equation, all modeling error occurs in matching the specified boundary conditions. The approximate boundary is the focus of points where the CVBEM model achieves the desired boundary values. Consequently, should the approximate boundary coincide with the true problem boundary, the CVBEM model is the exact solution to the boundary value problem. Equivalently, the error of approximation is visually demonstrated by the departure between the approximate and problem boundaries.

CVBEM DEVELOPMENT

For steady-state flow conditions, groundwater flow in a saturated, homogeneous, isotropic aquifer is mathematically modeled by the Laplace equation. The CVBEM has been shown to be a powerful numerical technique for the approximation of properly posed boundary-value problems involving the Laplace equations.[3] The keystone of the numerical approach is the integral function:

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

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. The function $G(\zeta)$ is a global trial function which is continuous on Γ. For example, given m nodal points specified on Γ defined by co-ordinates z_j, $j = 1, 2, \ldots, m$, let $\bar{\omega}_j$ be notation for the nodal values at node j. Then the m nodes result in m boundary elements Γ_j, $j = 1, 2, \ldots, m$ where Γ_j is the straight-line segment between co-ordinates z_j and z_{j+1} (Fig. 1). A linear global trial function is defined by:

$$G(\zeta) = \sum_{j=1}^{m} \delta_j (N_j \bar{\omega}_j + N_{j+1}\bar{\omega}_{j+1}) \tag{2}$$

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. In the above, the index situation of $j = m$ implies that index $(j+1)$ is equal to index 1. From the definition of $G(\zeta)$ we have:

$$\int_{\Gamma} \frac{G(\zeta)\,d\zeta}{\zeta - z} = \int_{\cup\Gamma_j} \frac{G(\zeta)\,d\zeta}{\zeta - z} = \sum_{j=1}^{m} \int_{\Gamma_j} \frac{G(\zeta)\,d\zeta}{\zeta - z}$$

$$= \sum_{j=1}^{m} \int_{\Gamma_j} \frac{(N_j\bar{\omega}_j + N_{j+1}\bar{\omega}_{j+1})\,d\zeta}{\zeta - z} \tag{3}$$

The CVBEM continues by using (3) 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. Given m nodes specified on Γ_j, we necessarily know either $\bar{\phi}$ or $\bar{\psi}$ (not both) at each z_j, $j = 1, 2, \ldots, m$. Then to estimate the remaining m nodal values, $\hat{\omega}(z)$ is collocated in the form of a Fredholm equation by forcing:

Class I:

$$\bar{\phi}_k(z_j) = \operatorname{Re}\hat{\omega}(z_j)$$
$$\bar{\psi}_k(z_j) = \operatorname{Im}\hat{\omega}(z_j) \tag{4a}$$

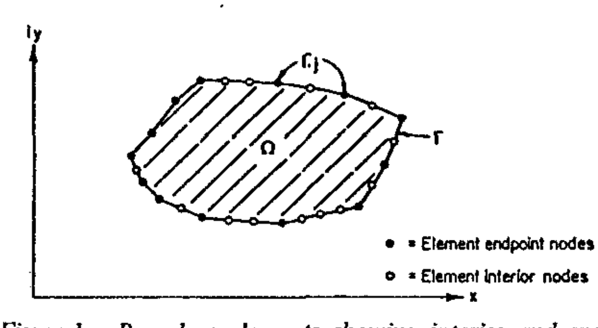

Figure 1. Boundary elements showing interior and endpoint nodes

Class II:

$$\bar{\phi}_u(z_j) = \text{Re}\ \hat{\omega}(z_j)$$
$$\bar{\psi}_u(z_j) = \text{Im}\ \hat{\omega}(z_j) \tag{4b}$$

In the above, the subscript u and k refer to unknown and known boundary condition nodal values, respectively. Because $\hat{\omega}(z_j) = \hat{\omega}(\bar{\phi}_k, \bar{\phi}_u, \bar{\psi}_k, \bar{\psi}_u)$, then a $\hat{\omega}(z)$ is determined by either (4a) or (4b) for $j = 1, 2, \ldots, m$. The difference between these two approximations is that the Class I system results in a CVBEM approximator which matches all the known nodal-point boundary-condition values, whereas the Class II system results in an approximation which equals the CVBEM-estimated unknown nodal-point boundary-condition values.

Because $G(\zeta)$ is continuous on each Γ_j, then $\hat{\omega}(z)$ is analytic for all $z \in \Omega$. Thus $\hat{\omega}(z)$ can be written as the sum of two harmonic conjugate functions by $\hat{\omega}(z) = \hat{\phi}(z) + i\hat{\psi}(z)$. Both the approximation functions, $\hat{\phi}(z)$ and $\hat{\omega}(z)$, satisfy the Laplace equation exactly for any $z \in \Omega$.

The modeling approach is to match the boundary conditions continuously on Γ. That is, we know values of ϕ or ψ at each nodal point z_j (thus we also know either ϕ or ψ continuously along each Γ_j). However, the CVBEM Class I approximator generally only equals the boundary conditions at nodal points where the Class II system results in a $\hat{\omega}(z)$ which may not equal a boundary condition value at any nodal point. If $\hat{\omega}(z)$ equals the boundary conditions continuously on Γ, then $\hat{\omega}(z)$ is the exact solution to the boundary-value problem.

Nodal equations are determined by taking the limit as the point $z \in \Omega$ approaches a selected nodal point $z_j \in \Gamma$ by:

$$\hat{\omega}(z_j) = \lim_{z \to z_j} \frac{1}{2\pi i} \int_\Gamma \frac{G(\zeta)\,d\zeta}{\zeta - z} \tag{5}$$

The limiting value is also known as the Cauchy principal value, and by using either the Class I or Class II systems, a set of m equations results; these equations are solvable for the unknown nodal values by the usual matrix-solution techniques such as Gaussian elimination.

FLOW FIELD MODEL DEVELOPMENT

The CVBEM is used to develop a potential function $F(z)$ which exactly satisfies the Laplace equation in Ω by:

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

where Q_i is the discharge from well i (of n) located at z_i (i.e. a sink); T is the transmissivity of a confined aquifer, and $\hat{\omega}(z)$, representing the background flow, is a CVBEM approximator developed for Ω. It is noted that $F(z)$ is subject to the boundary conditions:

$$\xi(z) = \delta\phi(z) + i(1 - \delta)\,\psi(z), \quad z \in \Gamma \tag{7}$$

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.

But the source and sink collection included in (6) represents an exact representation of the steady-state flow condition. Thus, $\xi(z)$ must be modified in order to develop a $\hat{\omega}(z)$ on Ω by:

$$\xi^*(z) = \xi(z) - \sum_{i=1}^{n} \frac{Q_i}{2\pi T} \ln(z - z_i), \quad z \in \Gamma \tag{8}$$

Thus, the flow field representation is developed by collocating $\hat{\omega}(z)$ at each node $z_j \in \Gamma$ according to the boundary-condition distribution of $\xi^*(z)$. The resulting approximation $F(z)$ describes the CVBEM numerical model. In (8), $\xi^*(z)$ is defined according to the real and imaginary parts as given in (7).

POISSON EQUATION

Given a continuous distribution of sources (such as from precipitation) or sinks in a flow field in domain Ω, the steady-state flow model of the Laplace equation must be extended to the Poisson equation:

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = k \tag{9}$$

where ϕ is the flow potential. Equation (9) can be modeled by choosing a particular solution ϕ_p such that:

$$\frac{\partial^2\phi_p}{\partial x^2} + \frac{\partial^2\phi_p}{\partial y^2} = k \tag{10}$$

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

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

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

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

The above procedure is extended to an arbitrary relation of the form:

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

by choosing a ϕ_p such that (13) is satisfied, and proceeding with the development of a suitable $\hat{\omega}(z)$ as described in the discussion leading to (12).

SOLUTE TRANSPORT

The solute-transport mechanism assumed is only applicable to the modeling of steady-state, advective contaminants, or 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:

$$\phi(z) = \text{Re}\,F(z) \tag{14}$$

In (14), $\text{Re}\,F(z)$ is the real part of the CVBEM approximator defined on Ω. The extent or boundary of the subsurface contamination is then redefined according to the point values of the flow velocity and the time increment selected before re-evaluation from the flow velocity field. Thus:

$$u = \frac{-\partial\phi}{\partial x} \Big/ \theta_0 \tag{15a}$$

$$v = \frac{-\partial\phi}{\partial y} \Big/ \theta_0 \tag{15b}$$

where (u, v) are (x, y)-direction specific discharges (or seepage velocities); and θ_0 is the saturated water content or porosity of the aquifer material. (A retardation factor, r, can be included in the denominator of (15) in order to account for contaminant-transport velocities being less than the actual fluid velocity or specific discharge.) The derivatives of (15) may be estimated as a finite difference of state variable values in the x and y directions, respectively.

The velocity of a contaminant particle is used to estimate the displacement with respect to time by setting:

$$\frac{dx^*}{dt} = u \tag{16a}$$

$$\frac{dy^*}{dt} = v \tag{16b}$$

where (x^*, y^*) are the co-ordinates of the subject contaminant particle. Integration of (16) with respect to time determines the pointwise displacement of a traced contaminant particle.

CVBEM MODELING-ERROR ANALYSIS

The specified boundary conditions are values of either constant ϕ or ψ on each Γ_j. These values correspond to level curves of the analytic function $\omega(z) = \phi + i\psi$. After developing a CVBEM approximation $\hat{\omega}(z)$, an approximate boundary $\hat{\Gamma}$ can be determined which corresponds to the level curves of $\hat{\omega}(z) = \hat{\phi} + i\hat{\psi}$ which equal the prescribed boundary conditions on Γ. Use of the Class I system is preferable due to $\hat{\Gamma}$ intersecting Γ at each nodal point. The resulting contour $\hat{\Gamma}$ is a visual representation of approximation error, and $\hat{\Gamma}$ coincident with Γ implies that $\hat{\omega}(z) = \omega(z)$. Additional collocation points are located in regions where $\hat{\Gamma}$ deviates substantially from Γ.

A difficulty in using this method for locating additional collocation points is that the contour $\hat{\Gamma}$ cannot be determined for points z outside of $\Omega \cup \Gamma$ by using $\hat{\omega}(z)$ as defined by (1). Thus, an analytic continuation of $\hat{\omega}(z)$ to the exterior is achieved by rewriting the integral function (a) as:

$$\frac{1}{2\pi i}\int_{\Gamma}\frac{G(\zeta)\,d\zeta}{\zeta - z} = R_1(z) + \sum_{j=1}^{m}(\alpha_j + i\beta_j)(z - z_j)\ln(z - z_j) \tag{17}$$

where α_j and β_j are real numbers; and $\ln(z - z_j)$ is a principal-value logarithm with branch-cuts drawn approximately normal to Γ from each branch point z_j such as shown in Fig. 2. The resulting approximation is analytic everywhere except along each branch-cut. The $R_1(z)$ function in equation (17) is a first-degree reference polynomial which results to the integration circuit of 2π radians along Γ. If $\omega(z)$ is not a first-degree polynomial (or a linear equation), then the $R_1(z)$ can be omitted.

Our strategy for determining the location of $\hat{\Gamma}$ is to subdivide each Γ_j with several internal points (about 4 to 6) and determine $\omega(z)$ at each point. Next, $\hat{\Gamma}$ is located by a Newton-Raphson stepping procedure in locating where $\hat{\omega}(z)$ matches the prescribed level curve. Thus, several evaluations of $\hat{\omega}(z)$ are needed to locate a single $\hat{\Gamma}$ point. The end product, however, may be considered very useful since it can be argued that $\hat{\omega}(z)$ is the exact solution to the boundary value problem with Γ transformed to $\hat{\Gamma}$, and $\hat{\Gamma}$ is a visual indication of approximation error.

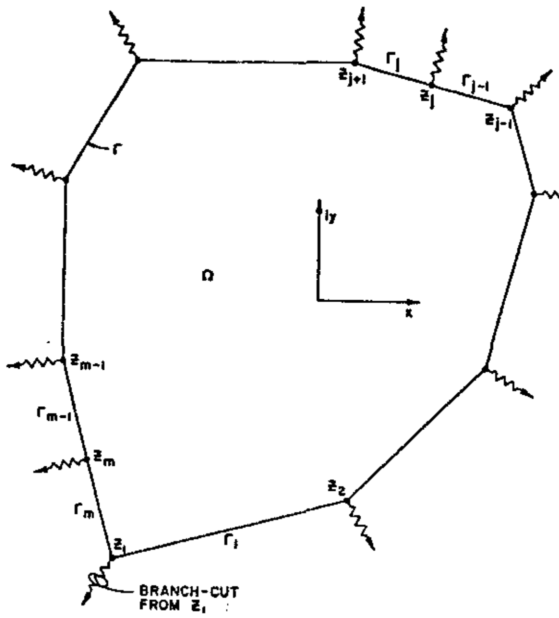

Figure 2. The analytic continuation of $\hat{\omega}(z)$ to the exterior of $\Omega \cup \Gamma$. (Note branch cuts along Γ at nodes z_j)

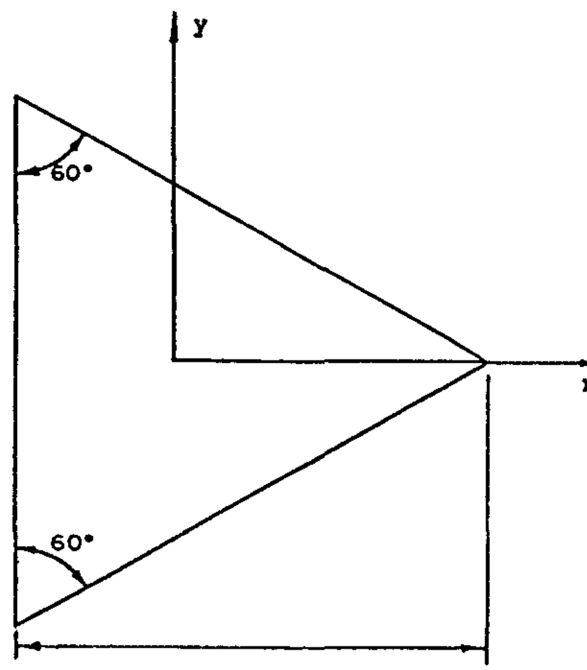

Figure 3. Triangle domain (potential problem)

For example, Fig. 3 shows a triangle domain with a specific local co-ordinate system. The CVBEM can be used to model the Laplace equation with boundary conditions for the potential given by:

$$\phi(z \in \Gamma) = \tfrac{1}{2}(x^2 + y^2) \tag{18}$$

The approximate boundary $\hat{\Gamma}$ is determined by location of the locus of points where:

$$\hat{\phi}(z) = \tfrac{1}{2}|z|^2 \tag{19}$$

Figure 4 shows three approximate boundaries corresponding to 6, 12, and 38 nodal points on Γ where nodes are

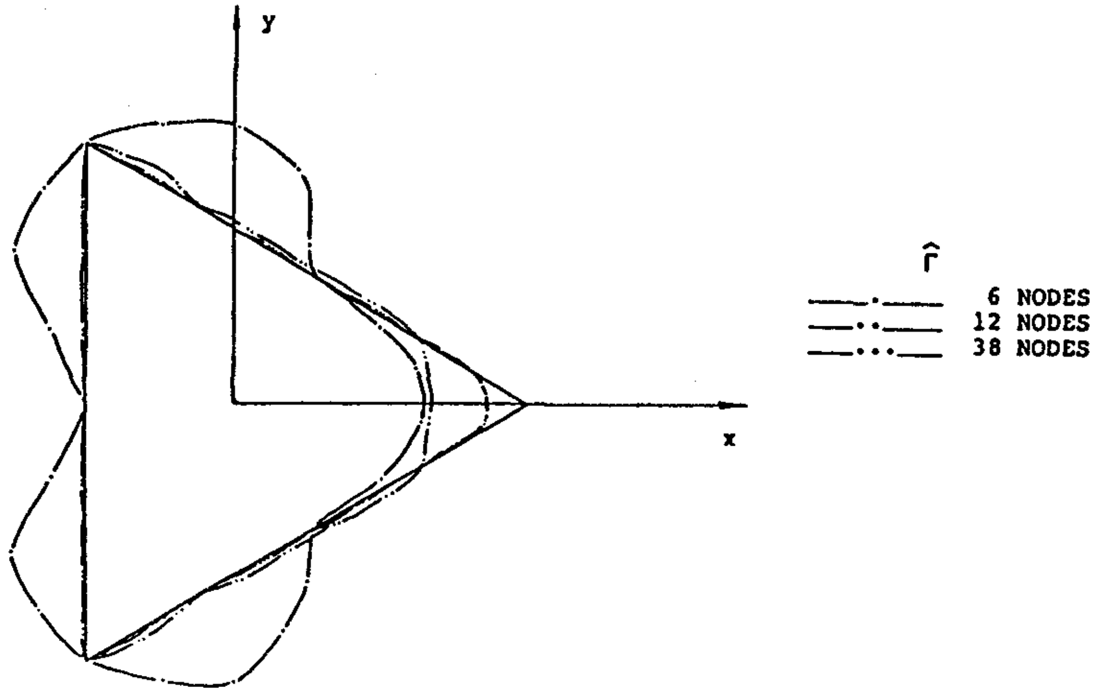

Figure 4. Approximate boundaries for three nodal points distributions

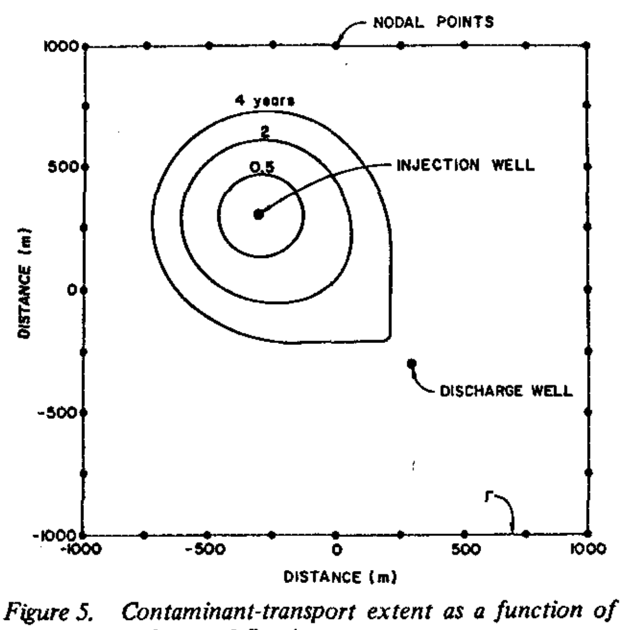

Figure 5. Contaminant-transport extent as a function of time (zero background flow)

located according to maximum departures between Γ and $\hat{\Gamma}$. Complete details of the approximate boundary technique are given in Hromadka.[3]

APPLICATION

As sample applications of the CVBEM technique to a combination of Laplacian and Poisson flows that may include the background flow and sources and sinks, the problem presented in Javandel *et al.*[2] is studied. Figure 5 shows a completely penetrating groundwater well (discharge 50 m^3/h) located in a homogeneous isotropic aquifer of thickness 10 m. Contaminated water is being recharged (recharge of 50 m^3/h) at another well located 848.5 m distance from the supply well. Effective porosity is 0.25, and negligible background groundwater flow is assumed. Retardation is assumed to be 1. CVBEM modeling results are based on the solution of (12).

Shown in Fig. 5 are the limits of groundwater contamination corresponding to model times of 0.5, 2, and 4 years. The predicted locations of the contaminant closely agree with the results given in Javendal *et al.*[2] (not shown). Additionally, the CVBEM model predicts a first arrival of con-

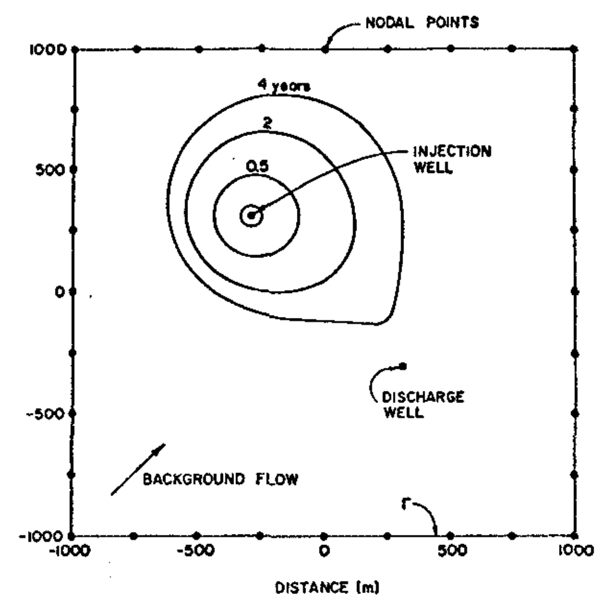

Figure 6. Contaminant-transport as a function of time (45° background flow)

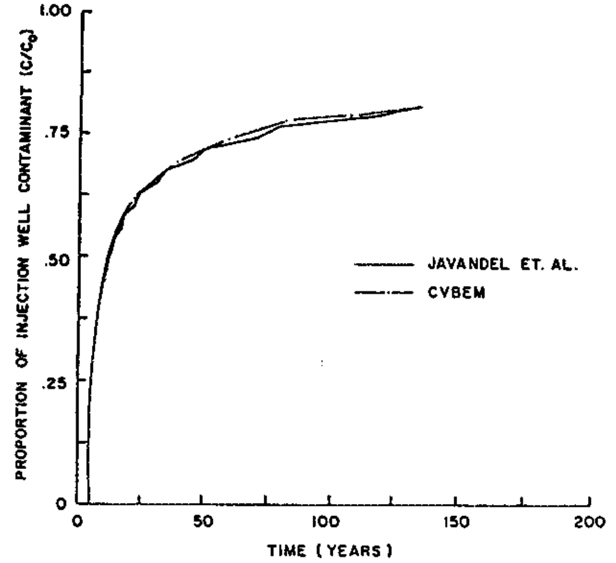

Figure 7a. Arrival of contaminant at the discharge well (case study 1)

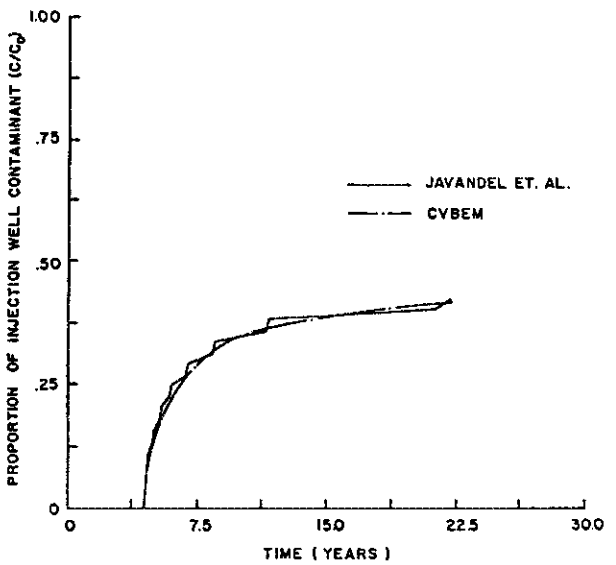

Figure 7b. Arrival of contaminant at the discharge well (case study 2)

tamination of time 4.4 years which agrees well with the Javendal estimate of arrival time (4.3 years) for injected water to reach the pumping site.

Figure 6 shows the problem of Fig. 5 restudied with the condition that a uniform background groundwater flow is evident at a 45° inclination, and a flow rate of fluid is 50 m/yr. In this study, the arrival time of contaminant is slowed to 4.7 years.

In both cases, the quantity of the arriving contamination versus time is estimated by simply integrating between the stream-function $\psi(z)$ values according to the contaminant arrival times (see (16)). A comparison of the quasi-analytic estimate of contamination arrival[2] to the CVBEM estimates are given in Fig. 7 for both case studies.

It is noted that the CVBEM model reduces to the quasi-analytic approach for the simple case studies considered. With considerations of local anisotropy and nonhomogeneity, and CVBEM technique provides means for a significant extension of the above quasi-analytic approach, enabling this comprehensive study method to be applied to a much larger class of problems.

SUMMARY AND CONCLUSIONS

Among many applications, the CVBEM can also be used to develop a model of steady-state, advective, contaminant transport in groundwater. 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. This modeling error analysis by means of constructing an approximate error analysis by means of constructing an approximative boundary where the CVBEM approximation satisfies the boundary conditions.

The presented model considers steady-state conditions for two-dimensional groundwater flows. The modeling technique is not applicable to three-dimensional problems. However, the modeling approach can be extended to include various steady-state boundary conditions, regional nonhomogeneity and anisotropy, and point or distributed sources and sinks.

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 microcomputers.

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