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Computer Modeling of Groundwater Contaminant Transport Using Complex Variable Approximations

T.V. Hromadka, II
C.C. Yen
Williamson and Schmid
Irvine, California

ABSTRACT

Recently advanced techniques in modeling groundwater contaminant transport include Boundary Element Methods and the more recent Complex Variable Boundary Element Method (CVBEM). In this paper, the CVBEM is reviewed and then applied to a suite of practical case studies. Problems considered include contaminant transport between contaminant sources and pumping wells, landfill sites and pumping wells, and the influence of injection wells on contaminant transport. Determination of flow-fields about protected barriers is examined. These recent numerical advances suggest future promise in the use of computer modeling techniques to develop solutions for mitigating contaminant transport.

INTRODUCTION

Mathematical modeling techniques which have been developed to predict the extent of subsurface contamination of groundwater 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 modeling category 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 quickly passes between the modeling categories.

For simple time-dependent solute transport within a domain which includes steady and uniform groundwater flow, analytical solutions are available for several one-dimensional or radial flow scenarios. For example, Van Genuchten and Alves¹ summarize the mathematical solutions to several one-dimensional convective-dispersive solute transport problems. Generally, such mathematical solutions are based on limited groundwater 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 groundwater 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.

For problem scenarios where the groundwater 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 scenarios where time-dependent boundary conditions and dispersion and diffusion effects are significant, the minimum modeling sophistication needed 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 modeling 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. Consequently, flow conditions and desired contaminant transport mechanisms can be modeled by the incorporation of various flow submodels or bookkeeping algorithms which simulate particular transport processes.

Associated with numerical methods are the complication of calibration of the model to meet known physical conditions and the potential for numerical approximation 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 approaches only satisfy the governing steady-state flow equations for basic scenarios such as uniform flow. Consequently, when using numerical methods, one must pay attention to numerical stability, choice of discretization, timestep advancement, timestep size and the overall accuracy of the coupled numerical models.

Various domain numerical models are available which include submodels for accommodating particular transport processes. A detailed tabulation of 32 such domain models is given in Javandel et al.,² which itemizes the numerical modeling approach, ancillary submodels and included transport processes.

A new direction for subsurface contaminant transport modeling is the use of the complex variable boundary element method or CVBEM.² 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 and can include spatially distributed sources and sinks such as mathematically described by Poisson's Equation.

For steady-state, two-dimensional problems, the CVBEM develops an approximation function which exactly solves the governing groundwater flow equation (Laplace Equation) within each homogeneous domain. For unsteady 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 by Hromadka² or Brebbia.¹ A new development from this paper will be the solution of the Poisson Equation in a homogeneous domain; this calculation will be the first time that the CVBEM has been applied to this class of partial differential equations.

Application of the CVBEM contaminant transport model is currently restricted to steady-state flow field scenarios where solute transport is water-coincident. That is, mass transport by diffusion and dispersion is not included. However, it is noted that the CVBEM model requires only a limited amount of data and does not require the discretization of the domain into a mesh or set of control volumes or 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 using an approximative 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 approximative boundary is the locus of points where the CVBEM model achieves the desired boundary values. Consequently, should the approximative 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 approximative 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 Equation.² The keystone of the numerical approach is the integral function:

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

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 coordinates $z_j, j = 1, 2, \dots, m$, let ω_j be notation for the nodal values at node j . Then the m nodes result in m boundary elements $\Gamma_j, j = 1, 2, \dots, m$ where Γ_j is the straight line segment between coordinates z_j and z_{j+1} (Figure 1). A linear global trial function is defined by:

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

where $\delta_j = 1$ if $\zeta \in \Gamma_j$, and $\delta_j = 0$ if $\zeta \in \Gamma_j$. 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:

$$\int_{\Gamma} \frac{G(\zeta) d\zeta}{\zeta - z} = \int_{\Gamma_1} \frac{G(\zeta) d\zeta}{\zeta - z} + \dots + \int_{\Gamma_j} \frac{G(\zeta) d\zeta}{\zeta - z} + \dots + \int_{\Gamma_m} \frac{G(\zeta) d\zeta}{\zeta - z} = \sum_{j=1}^m \int_{\Gamma_j} \frac{(N_j \bar{\omega}_j + N_{j+1} \bar{\omega}_{j+1}) d\zeta}{\zeta - z} \quad (3)$$

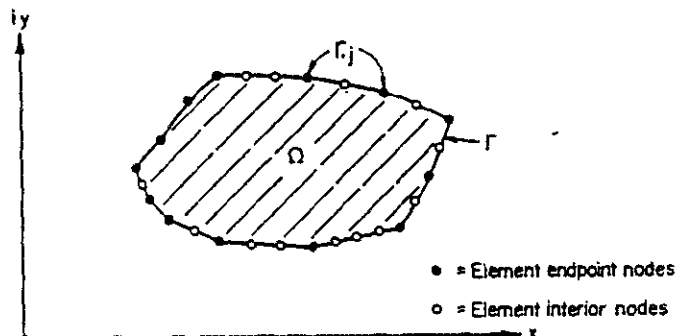


Figure 1
Boundary Elements
Showing Interior and End-point Nodes

The CVBEM continues by using Equation 3 to develop m equations as a function of the m unknowns associated with the undetermined nodal values of either ϕ or ψ at each node. That is, $\omega = \phi + i\psi$ where ϕ and ψ are nodal values of the potential and stream functions, respectively. Given m nodes specified on $\Gamma_j, j = 1, 2, \dots, m$, we necessarily know either ϕ or ψ (not both) at each $z_j, j = 1, 2, \dots, m$. To estimate the remaining m nodal values, $\omega(z)$ is collocated in the form of a Fredholm Equation by forcing:

$$\begin{aligned} \text{CLASS I:} \quad \bar{\phi}_k(z_j) &= \text{Re } \hat{\omega}(z_j) \\ \bar{\psi}_k(z_j) &= \text{Im } \hat{\omega}(z_j) \end{aligned} \quad (4a)$$

$$\begin{aligned} \bar{\phi}_U(z_j) &= \text{Re } \hat{\omega}(z_j) \\ \bar{\psi}_U(z_j) &= \text{Im } \hat{\omega}(z_j) \end{aligned} \quad (4b)$$

In the above equations, the subscript U and k refer to unknown and known boundary condition nodal values, respectively. Because $\omega(z) = \omega(\phi_k, \phi_U, \psi_k, \psi_U)$, then a $\omega(z)$ is determined by either Equation 4a or 4b for $j = 1, 2, \dots, m$. 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 , $\omega(z)$ is analytic for all $z \in \Omega$. Thus $\omega(z)$ can be written as the sum of two harmonic conjugate functions by $\omega(z) = \phi(z) + i\psi(z)$. Both the approximation $\phi(z)$ and $\psi(z)$ functions 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, whereas the class II system results in a $\omega(z)$ which may not equal a boundary condition value at any nodal point. If $\omega(z)$ equals the boundary conditions continuously on Γ , then $\omega(z)$ 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:

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

The limiting value is also the Cauchy principle value, and by using either the class I or class II systems, a set of m equations result which 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:

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

where Q_i is the discharge from well i (of n) located at z_i and $\omega(z)$ is a CVBEM approximator developed for Ω . It is noted that $F(z)$ is subject to the boundary conditions:

$$\xi(z) = \Delta\phi(z) + i(1-\Delta)\psi(z), \quad z \in \Gamma \quad (7)$$

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 Equation 6 represents an exact representation of the steady-state flow condition. Thus, $\xi(z)$ must be modified in order to develop a $\omega(z)$ on Ω by:

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

Thus, the flow field representation is developed by collocating $\omega(z)$ 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 Equation 8, $\xi^*(z)$ is defined according to the real and imaginary parts as given in Equation 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:

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

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

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

For example, $\phi_p = k/2(x^2 + y^2)$ 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 $\omega(z)$ on Ω by:

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

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

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

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

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

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

SOLUTE TRANSPORT

The solute transport mechanism assumed is only applicable to the modeling of steady-state, fluid-coincident 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:

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

In Equation 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 reevaluation from the flow velocity field. Thus:

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

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

where (u, v) are (x, y) -direction specific discharges, 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 Equation 15 in order to account for contaminant transport velocities being less than the actual fluid velocity or specific discharge.)

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

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

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

where (x^*, y^*) are the coordinates of the subject contaminant particle. Integration of Equation 16 with respect to time determines the pointwise rate of 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 approximative boundary Γ can be determined which corresponds to the level curves of $\hat{\omega}(z) = \phi + i\psi$ which equal the prescribed boundary conditions on Γ . Use of the class I system is preferable due to Γ intersecting Γ at each nodal point. The resulting contour Γ is a visual representation of approximation error, and Γ coincident with Γ implies that $\omega(z) = \hat{\omega}(z)$. Additional collocation points are located at regions where Γ deviates substantially from Γ .

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

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

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

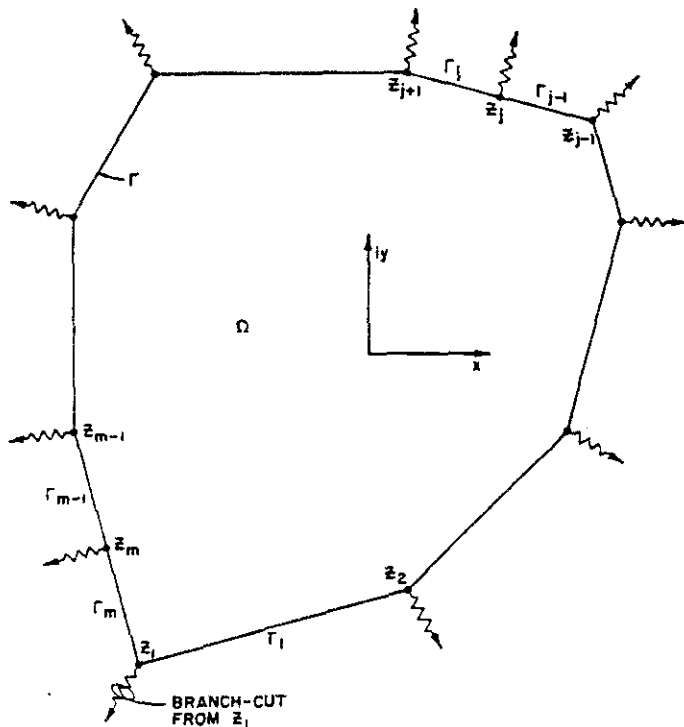


Figure 2

The Analytic Continuation of $\omega(z)$ to the Exterior of $\Omega \cup \Gamma$.
Note Branch cuts along Γ at nodes z_j .

One strategy for determining the location of Γ is to subdivide each Γ_j with several internal points (approximately 4 to 6) and determine

$\omega(z)$ at each point. Next, Γ is located by a Newton-Raphson stepping procedure in locating where $\omega(z)$ matches the prescribed level curve. Thus, several evaluations of $\omega(z)$ are needed to locate a single Γ point. The end-product, however, may be considered very useful since it can be argued that $\omega(z)$ is the exact solution to the boundary value problem with Γ transformed to Γ , and Γ is a visual indication of approximation error.

For example, Figure 3 shows a triangle domain with a specific local coordinate system. The CVBEM can be used to model the Laplace Equation with boundary conditions for the potential given by:

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

The approximative boundary Γ is determined by location of the locus of points where:

$$\hat{\phi}(z) = \frac{1}{2} |z|^2 \quad (19)$$

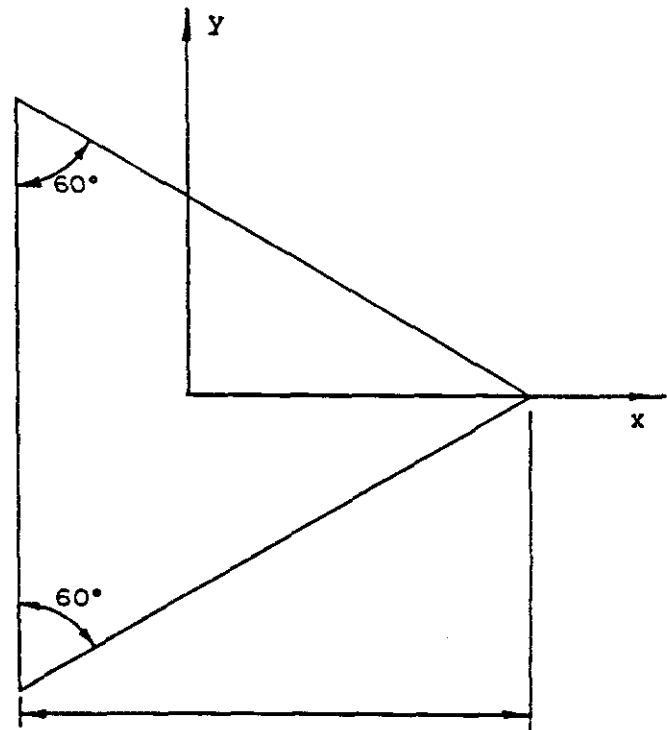


Figure 3

Triangle Domain (Potential Problem)

Figure 4 shows three approximative boundaries corresponding to 6, 12 and 38 nodal points on Γ where nodes are located according to maximum departures between Γ and Γ .

APPLICATION

As an example application of the CVBEM technique, the problem presented in Javandel et al.³ is studied. Figure 5 shows a completely penetrating groundwater well (discharge $50 \text{ m}^3/\text{hr}$) located in a homogeneous isotropic aquifer 10 m thick. Contaminated water is being recharged (recharge of $50 \text{ m}^3/\text{hr}$) at another well located 848.5 m from the supply well. Effective porosity is 0.25, and negligible background groundwater flow is assumed. Retardation is assumed to be unity.

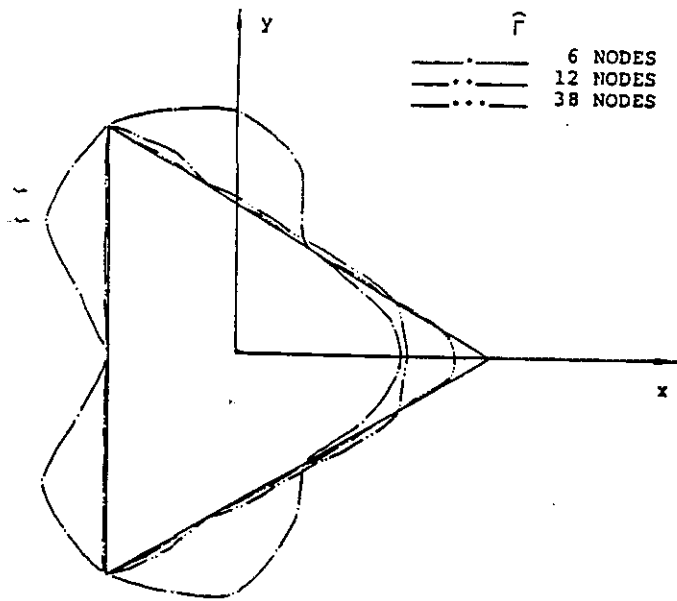


Figure 4
Approximate Boundaries for Three Nodal Point Distributions

a 45° inclination, and a flowrate of fluid is 50 m/yr. In this study, the arrival time of contaminant is slowed to 4.7 years.

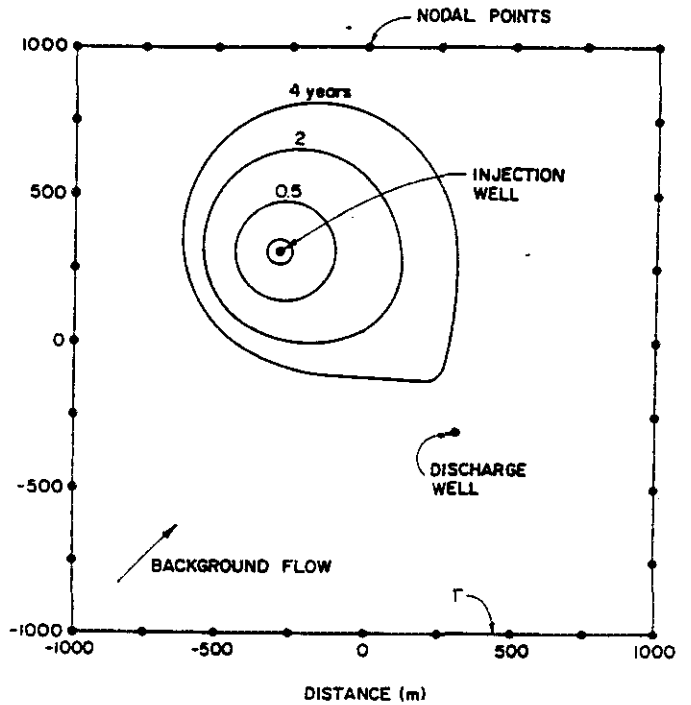


Figure 6
Contaminant Transport as a Function of Time (45° Background flow)

In both cases, the quantity of contamination arriving versus time is estimated by simply integrating between the stream function $\psi(z)$ values according to the contaminant arrival times. A comparison of the quasi-analytic estimate of contamination arrival³ to the CVBEM estimates is given in Figure 7 for both case studies.

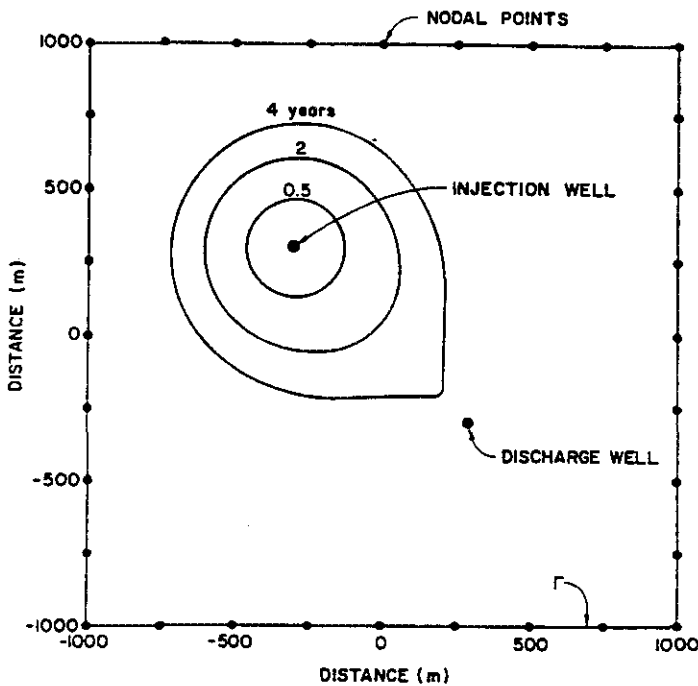


Figure 5
Contaminant Transport Extent As a Function of Time (Zero Background Flow)

Shown in Figure 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 Javandel et al.³ (not shown). Additionally, the CVBEM model predicts a first arrival of contamination at time 4.4 years which agrees well with the Muskat estimate of arrival time (4.3 years) for injected water to reach the pumping site.⁴

Figure 6 shows the problem of Figure 5 restudied with the condition that a uniform background groundwater flow is evident at

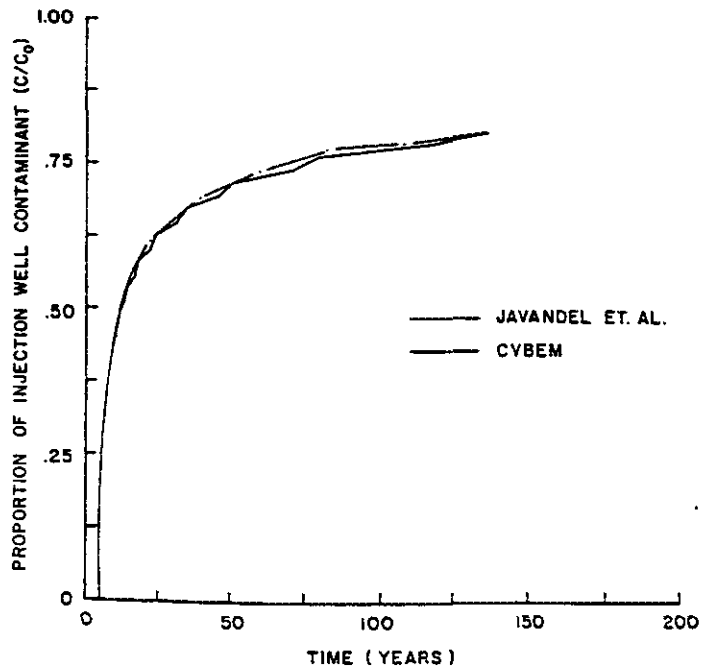


Figure 7a
Arrival of Contaminant at the Discharge Well. (Case Study 1)

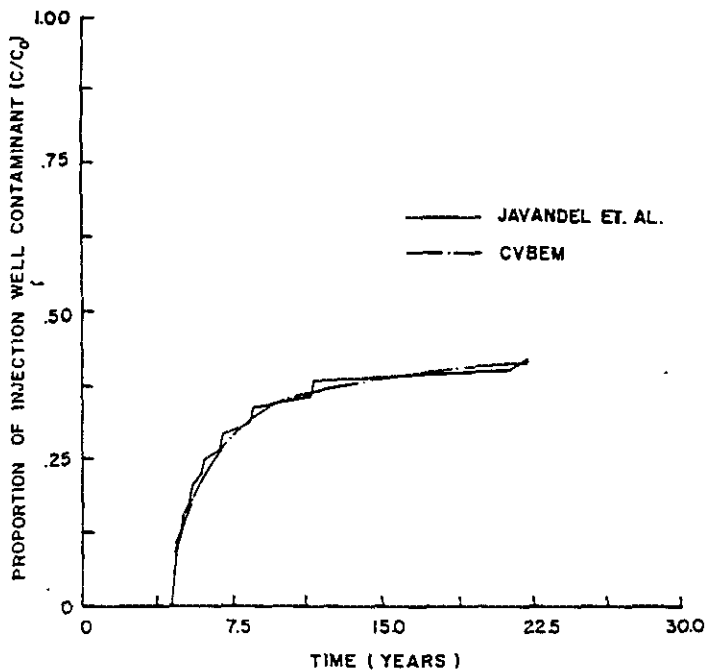


Figure 7b
Arrival of Contaminant at the Discharge Well. (Case Study 2)

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

CONCLUSIONS

The CVBEM can be used to develop a model of steady-state, fluid-coincident, contaminant transport in groundwater. Because the CVBEM provides approximations which exactly solve the Laplace and Poisson partial differential equations, all modeling error occurs in matching the prescribed boundary conditions. This modeling error, in turn, is subject to a direct and easily interpretable error analysis by constructing an approximative boundary where the CVBEM approximation satisfies the boundary conditions.

The presented model considers steady-state conditions for two dimensional scenarios. The modeling technique is not extendable to three-dimensional problems. However, the modeling approach can 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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