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The Complex Variable Boundary Element Method in Groundwater Contaminant Transport

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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.

In this paper, only the steady-state, two-dimensional, advection transport flow problem will be considered. The applications include the background flows, sources and sinks, and flows introduced by the boundary conditions. The numerical analogy produces locations of streamlines and the time-evolution of the contaminant front location. Due to the small coding requirements, the CVBEM program is operable on a typical home computer.

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 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 Poisson's equation. Detail developments of the CVBEM numerical technique are given in Hromadka [1984a and b].

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 $\vec{V}$ 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's 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.

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

CVBEM Development

The CVBEM has been shown to be a powerful numerical technique for the approximation of properly posed boundary-value problems involving the Laplace equation (Hromadka, 1984b). The keystone of the numerical approach is the integral function

$$\hat{\omega}(z) = \frac{1}{2\pi i} \int_{\Gamma} \frac{G(\zeta)\, d\zeta}{\zeta - z} \tag{6}$$

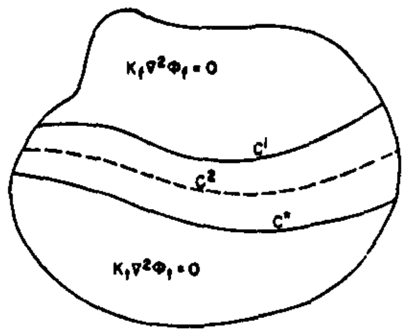

Fig.1. Iterative Estimation of Freezing Front Location

The third iteration step proceeds by defining Ω_f^3 and Ω_t^3 based on the mutual boundary of C^2 and the above procedure is repeated.

The iteration process continues until the final estimates of Ω_f and Ω_t are determined with corresponding $\hat{\omega}_f$ and $\hat{\omega}_t$ approximators such that

$$|k_f d\hat{\psi}_f/ds - k_t d\hat{\psi}_t/ds| < \varepsilon, \ z \ \varepsilon C \tag{2}$$

<u>Using the Approximate Boundary</u>

As discussed previously, the subject problem reduces to finding a solution to the Laplace equation in Ω_f and Ω_t where Ω_f and Ω_t coincide along the steady state freezing front location, C. The CVBEM develops approximators ω_f and $\hat{\omega}_t$ which satisfy the Laplace equation over Ω_f and Ω_t, respectively. Consequently, the only numerical error occurs in matching the boundary conditions continuously on Γ_f, Γ_t, and C.

To evaluate the precision in predicting the freezing front location, an approximate boundary is determined for each subproblem domain of Ω_f, Ω_t. The approximate boundary results from plotting the level curves of each CVBEM approximator (i.e. $\hat{\omega}_f$, $\hat{\omega}_t$) which correspond to the boundary conditions of the problem.

For example, in Ω_f the thermal boundary conditions for a roadway embankment (Fig. 2) are defined on the problem boundary Γ_f by

$\phi = -10°C$, $z \ \varepsilon$ top surface

$\phi = 0°C$, $z \ \varepsilon$ freezing front

$\psi = 0$, $z \ \varepsilon$ left side (symmetry)

$\psi =$ constant, $z \ \varepsilon$ right side (zero flux)

After developing an $\hat{\omega}_f$ and Ω_f from the CVBEM, the approximate boundary $\hat{\Gamma}_f$ is determined by plotting the prescribed level curves. The figure also includes $\hat{\Gamma}_f$ superimposed with Γ_f. Because $\hat{\omega}_f$ is analytic within the interior of the approximate boundary and satisfies the prescribed boundary conditions on the boundary $\hat{\Gamma}_f$, then $\hat{\omega}_f$ is the exact solution of the boundary value problem

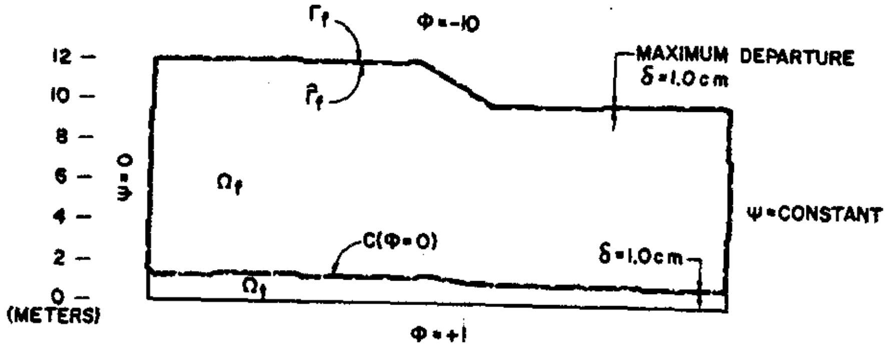

Fig. 2. The Approximate Boundary $\hat{\Gamma}_f$ and the closeness-of-fit to the Problem Boundary, Γ_f

redefined on $\hat{\Gamma}_f$ and its interior, $\hat{\Omega}_f$. Should $\hat{\Gamma}_f$ completely cover Γ_f, then $\hat{\omega}_f$ is the exact solution to the subject problem.

Thus, the CVBEM modeling error is directly evaluated by the closeness-of-fit between $\hat{\Gamma}_f$ and Γ_f. However in this application, the approximate boundary concept is used not only to examine the closeness-of-fit to the boundary conditions, but possibly more crucial, the closeness-of-fit of matching the estimated freezing front location between Ω_f and Ω_t along the contour, C. Should Ω_f and Ω_t match C continuously, then $\hat{\omega}_f$ and ω_t equate thermal flux continuously along C.

Applications

Figure 2 depicts an application of the geothermal model for a roadway embankment problem and the use of the approximate boundary. Figure 3 illustrates the two-dimensional steady state freezing front location for a geothermal problem involving a buried sub-freezing 3-meter diameter pipeline. An examination of the approximate boundaries indicate that a good CVBEM approximator was determined by use of a 26-node CVBEM model. The maximum departure δ between the approximate boundaries and the problem boundary Γ occurred along the top of the pipeline and had a value of approximately 3.5 cm. The average departure $\bar{\delta}$ is estimated at less than 1 cm. The freezing front maximum departure is approximately 4 cm and occurred at the right-hand side. Average departure on C is less than 2 cm.

The example problems presented illustrate the usefulness of the CVBEM in predicting the steady state freezing front location for two-dimensional problems. Possibly the most important result is the accurate determination of the approximation error involved in using the CVBEM. The usual procedure is estimating the freezing front is to use a finite element or finite difference numerical analog. A hybrid of these domain methods is to include a variable mesh in order to better accommodate the interface. However, none of these methods provide the error of approximation. In comparison, the CVBEM model provides the approximation error not only in matching the boundary conditions, but in predicting the interface location between Ω_f and Ω_t. And this error is simple to interpret

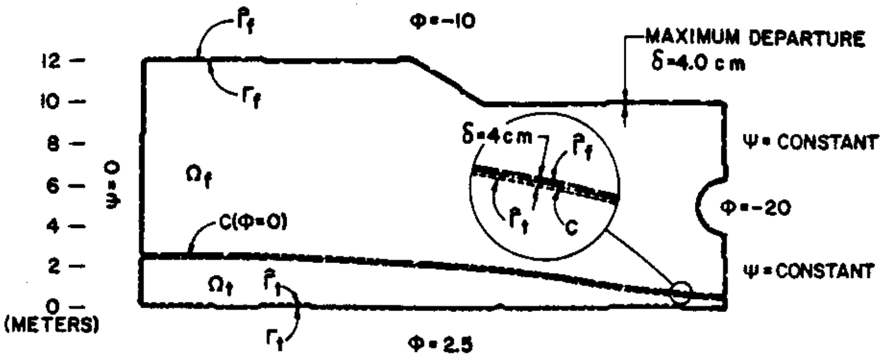

Fig. 3. Application of the CVBEM Geothermal Model to Predict Steady-State Conditions

as an approximate boundary displacement from the true problem boundary, and the displacement between Ω_f and Ω_t along the freezing front contour, C.

Time-stepped Approximate Boundary

By plotting the several CVBEM generated approximate boundaries, the time evolution of approximation error is readily seen. Figure 4 demonstrates the CVBEM modeling error in the time sequence of approximations developed for the pipe solution isolated from the Fig. 3 problem. From Fig. 4, it is concluded that the computational effort employed by the CVBEM analysis is adequate for this case study. The figure shows a variation in the approximate boundary location as the solution progresses in time; however, the variation is of less than 1.0 cm in magnitude.

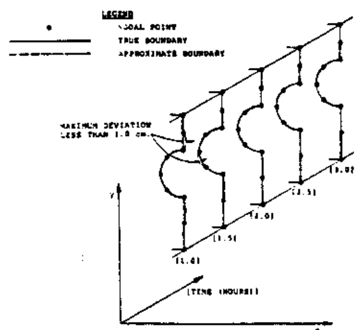

Fig. 4. Approximate Boundary Evolution for Time-Stepped Problem Solution (see Fig.3 for Domain Definition)

Conclusions

In this paper the CVBEM is used to approximate a slowly-moving interface between two quasi-potential problem solutions. The case study considered is soil-water phase change in freezing soils. The approximate boundary technique is used to demonstrate the CVBEM modeling error in achieving the prescribed boundary conditions as the time-stepped advancement in time is approximated.

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