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APPROXIMATION OF SLOW-MOVING INTERFACE PHASE CHANGE PROBLEMS USING A GENERALIZED FOURIER SERIES AND THE COMPLEX VARIABLE BOUNDARY ELEMENT METHOD

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Many important engineering problems fall into the category of linear operators, with supporting boundary conditions. In this paper a new inner product and norm are developed that enable the numerical modeler to approximate such engineering problems by developing a generalized Fourier series. The resulting approximation is the "best" approximation in that a least-squares (L^2) error is minimized simultaneously for fitting both the problem's boundary conditions and satisfying the linear operator relationship (the governing equations) over the problem's domain (both space and time). For slow-moving interface phase change problems where the heat flux balance can be adequately described by the Laplace equation, the generalized Fourier series technique results in a highly accurate solution.

INNER PRODUCTS FOR THE SOLUTION OF LINEAR OPERATOR EQUATIONS

The general setting for solving a linear operator equation with boundary values by means of an inner product is as follows. Let Ω be a region in R_m with boundary Γ and denote the closure of Ω by $\mathrm{cl}(\Omega)$. consider the Hilbert space $L^2(\mathrm{cl}(\Omega),d\mu)$, which has inner product $(f,g) = \int fg\, d\mu$. (This is a real Hilbert space. For the complex version, use the complex conjugate of the function g in the integral.) The way to construct the necessary inner product for the development of a generalized Fourier series is to choose the measure μ correctly; that is, let μ be one measure μ_1 on Ω and another meaure μ_2 on Γ. One natural choice for a plane region would be for μ_1 to be the usual two-dimensional Lebesgue measure dV on Ω and μ_2 the usual arc length measure ds on Γ. Then an inner product is given by [1]

$$(f,g) = \int_\Omega fg\, dV + \int_\Gamma fg\, ds \tag{1}$$

Consider a boundary-value problem consisting of an operator L defined on domain $D(L)$ contained in $L^2(\Omega)$ and mapping into $L^2(\Omega)$, and a boundary condition operator B defined on a domain $D(B)$ in $L^2(\Omega)$ and mapping into $L^2(\Gamma)$. The domains of L and B must be chosen so that at least for f in $D(L)$, Lf is in $L^2(\Omega)$, and for f in $D(B)$, Bf is in $L^2(\Gamma)$. For example, we could have $Lf = \nabla^2 f$ and $Bf(s)$ equal to the almost everywhere (a.e.) radial limit of f at the point s on Γ, with appropriate domains.

The next step is to construct an operator T, mapping its domain $D(T) = D(L) \cap D(B)$ into $L^2(\mathrm{cl}(\Omega))$ by (e.g., see [2])

$$\begin{aligned} Tf(x) &= Lf(x) \qquad \text{for } x \text{ in } \Omega \\ Tf(s) &= Bf(s) \qquad \text{for } s \text{ on } \Gamma \end{aligned} \tag{2}$$

From Eq. (2) there exists a single operator T on the Hilbert space $L^2(\mathrm{cl}(\Omega))$ that incorporates both the operator L and the boundary conditions B and is linear if both L and B are linear. An application of this procedure using the complex variable boundary element method (CVBEM) is given in Hromadka et al. [3]. In that study, $Lf = \nabla^2 f$ and Bf is the radial limit of f on Γ. Other applications are contained in Hromadka et al. [4, 5].

Consider the inhomogeneous equation $Lf = g_1$ with the inhomogeneous boundary conditions $Bf = g_2$. Then define a function g on $\mathrm{cl}(\Omega)$ by

$$\begin{aligned} g &= g_1 \qquad \text{on } \Omega \\ g &= g_2 \qquad \text{on } \Gamma \end{aligned}$$

Then if the solution exists for the operator equation

$$Tf = g$$

the solution f satisfies $\nabla^2 f = g_1$ on Ω, and $f = g_2$ on Γ in the usual sense of meaning that the radial limit of f is g_2 on Γ. One way to attempt to solve the equation $Tf = g$ is to look at a subspace D_n of dimension n, which is contained in $D(T)$, and try to minimize $\|Th - g\|$ over all the h in D_n as developed in Hromadka et al. [6].

Purpose of Paper

In this paper the mathematical development of the approximation procedure and the application of the technique to a heat transfer problem are presented.

A detailed derivation of the technique and the application to several simple problems are given in Hromadka et al. [4, 5]. Because this technique shows considerable promise in many engineering applications, the computational effort involved, which is greater than that needed with a finite-element or finite-difference method solution, may be offset by the mathematical attractiveness of a convergence (in the L^2 sense) that can be linearly programmed.

Definition of Inner Product and Norm

Given a linear operator relationship

$$L(\phi) = h \quad \text{on } \Omega, \qquad \phi = \phi_b \quad \text{on } \Gamma \tag{3}$$

defined on the problem domain Ω with auxiliary conditions of $\phi = \phi_b$ on the boundary Γ (see Fig. 1). Here Ω may represent both time and space, and ϕ_b may be both

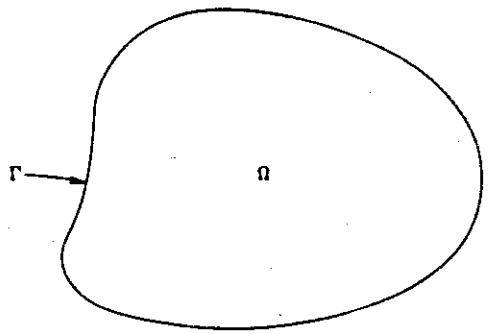

Fig. 1 Definition of problem domain Ω and boundary Γ. (Note: ϕ_b can include the temporal term boundary of the initial condition specification.)

initial and boundary conditions. It is assumed that the working space is sufficiently restricted (see below) that ϕ is a unique a.e. solution to Eq. (3).

Choose a set of m linearly independent functions $\langle f_j \rangle^m$, and let S^m be the m-dimensional space spanned by the elements of $\langle f_j \rangle^m$. Here the elements of $\langle f_j \rangle^m$ will be assumed to be functions of the dependent variables appearing in Eq. (3).

An inner product is defined for elements of S^m by (u,v), where for $u, v \in S^m$

$$(u,v) = \int_\Gamma uv \, d\Gamma + \int_\Omega LuLv \, d\Omega \tag{4}$$

It is seen that (u,v) is indeed an inner product, because for elements u, v, w in S^m

1. $(u,v) = (v,u)$
2. $(ku,v) = k(u,v)$ for L a linear operator
3. $(u + v,w) = (u,w) + (v,w)$ for L a linear operator
4. $(u,u) = \int_\Gamma (u)^2 \, d\Gamma + \int_\Omega (Lu)^2 \, d\Omega \geq 0$
5. $(u,u) = 0 \Rightarrow u = 0$ a.e. on Γ, and $Lu = 0$ a.e. over Ω

These restrictions on the operator L imply that L is linear (see parts 1 and 2 of the above definition); if $Lu = 0$ a.e. over Ω and $u = 0$ a.e. on Γ, this must imply that the solution $u = [0]$, where $[0]$ is the zero element over $\Omega \cup \Gamma$; and for the inner product to exist, the integrals must exist. For the inner product of Eq. (4) to exist, the integrands must be finite. In addition, each element $u \in S^m$ must satisfy $\int_\Gamma u^2 \, d\Gamma < \infty$.

For the above restrictions on L and the space S^m, the inner product is defined and a norm, $\| \ \|$, immediately follows:

$$\|u\| \equiv (u,u)^{1/2} \tag{5}$$

The generalized Fourier series approach can now be used to obtain the "best" approximation $\phi_m \in S^m$ of the function ϕ, using the newly defined inner product and corresponding norm presented in Eqs. (4) and (5).

The next step in developing the generalized Fourier series is to construct a new set of functions $\langle g_j \rangle^m$ that are the orthonormal representation of the $\langle f_j \rangle^m$.

Orthonormalization Process

The functions $\langle g_j \rangle^m$ can be obtained by the well-known Gramm-Schmidt procedure [7, p. 45], using the newly defined norm of Eq. (4). That is,

$$g_1 = \frac{f_1}{\|f_1\|}$$

$$\vdots \tag{6}$$

$$g_m = \frac{[f_m - (f_m,g_1)g_1 - \cdots - (f_m,g_{m-1})g_{m-1}]}{\|f_m - (f_m,g_1)g_1 - \cdots - (f_m,g_{m-1})g_{m-1}\|}$$

Hence, the elements of $\langle g_j \rangle^m$ satisfy the convenient properties that

$$(g_j,g_k) = \begin{cases} 0 & \text{if } j \neq k \\ 1 & \text{if } j = k \end{cases} \tag{7}$$

In a subsequent section a simple one-dimensional problem illustrates the orthonormalization procedure of Eq. (6).

The elements $\langle g_j \rangle^m$ also form a basis for S^m but, because of Eq. (7), can be directly used in the development of a generalized Fourier series where the computed coefficients do not change as the dimension m of $\langle g_j \rangle^m$ increases. That is, as the number of orthonormalized elements increases in the approximation effort, the previously computed coefficients do not change. Each element $\phi_m \in S^m$ can now be written as

$$\phi_m = \sum_{j=1}^{m} \gamma_j g_j \quad \phi_m \in S^m \tag{8}$$

where γ_j are unique real constants.

Generalized Fourier Series

The ultimate objective is to find the element $\phi_m \in S^m$ such that $\|\phi_m - \phi\|$ is a minimum. That is, we want $\|\phi_m - \phi\|^2$ to be a minimum, where

$$\|\phi_m - \phi\|^2 = \int_\Gamma \left(\sum_{j=1}^{m} \gamma_j g_j - \phi_b \right)^2 d\Gamma + \int_\Omega \left(L \sum_{j=1}^{m} \gamma_j g_j - L\phi \right)^2 d\Omega \tag{9}$$

Remembering that L is a linear operator and $L\phi = f$ by the problem definition of Eq. (3), we have that Eq. (9) can be rewritten as

$$\|\phi_m - \phi\|^2 = \int_\Gamma \left(\sum_{j=1}^{m} \gamma_j g_j - \phi_b \right)^2 d\Gamma + \int_\Omega \left(\sum_{j=1}^{m} \gamma_j L g_j - f \right)^2 d\Omega \tag{10}$$

Thus, minimizing $\|\phi_m - \phi\|^2$ is equivalent to minimizing the error or approximating

the boundary conditions and the error of approximating the governing operator relationship in a least-squares (or L^2) sense. Because the $\langle g_j \rangle^m$ are orthonormalized and the inner product (,) is well defined, the coefficients γ_j of Eq. (8) are immediately determined by the generalized Fourier constants γ_j^*, where

$$\gamma_j^* = (g_j, \phi) \qquad j = 1, 2, \ldots, m \tag{11}$$

Thus

$$\phi_m^* = \sum_{j=1}^{m} \gamma_j^* g_j = \sum_{j=1}^{m} (g_j, \phi) g_j \tag{12}$$

is the "best" approximation of ϕ, in the space S^m.

Because the generalized Fourier series approach is used, several advantages over a matrix solution (for the generalized Fourier series coefficients) are obtained:

1. The need to solve large, fully populated matrices, which arises when solving the normal equations, is eliminated.
2. The instability that typically arises in a matrix solution for Fourier coefficients (i.e., higher powers of the expansion basis functions assumed) is eliminated.
3. The generalized Fourier series coefficients do not change as additional functions are added (i.e., as the dimension m of the space S^m is increased).
4. Generalized Fourier series theory applies; hence, error analysis can be conducted using Bessel's inequality, as discussed in the next section.

Approximation Error Evaluation

Due to the generalized Fourier series approach and the definition of the inner product, Bessel's inequality applies. That is, for any dimension m

$$(\phi, \phi) \geq \sum_{j=1}^{m} (g_j, \phi)^2 = \sum_{j=1}^{m} \gamma_j^{*2} \tag{13}$$

where

$$(\phi, \phi) = \int_\Gamma (\phi)^2 \, d\Gamma + \int_\Omega (L\phi)^2 \, d\Omega = \int_\Gamma \phi^2 \, d\Gamma + \int_\Omega f^2 \, d\Omega \tag{14}$$

Equation (14) is readily evaluated and forms an upper bound to the sum of $(g_j, \phi)^2$ as the dimension m increases. Consequently, one may interact with the approximation effort by carefully adding functions to the $\langle f_j \rangle^m$ in order to best reduce the difference computed by Bessel's inequality. The technique of reducing Bessel's inequality can be linearly programmed by choosing additional basis functions that provide the greatest reduction in Eq. (13) from the set of basis functions available.

APPLICATION TO SLOW-MOVING INTERFACE PHASE PROBLEMS

Many freezing/thawing phase change situations fall in the category of heat transfer problems where the heat flux along the phase change boundary is adequately estimated by assuming the Laplace equation. For example, for soil-water phase change in freezing soils, Hromadka and Guymon [8] successfully used the Laplace equation to compute heat flux quantities along the freezing front of a soil column in order to propagate the front due to soil-water phase change. In another application, Hromadka [6] used the CVBEM to extend the soil-water phase change solution to two dimensions. A distinct advantage afforded by the CVBEM solution is the error analysis by use of the "approximate boundary" technique (see Hromadka [9]).

In this paper the CVBEM trial functions are used to eliminate the second integral in the inner product of Eq. (4). Thus,

$$(u,v) = \int_{\Gamma} uv \, d\Gamma \tag{15}$$

becomes the inner product for the generalized Fourier series development.

Modeling Approach

The modeling approach (the governing equations and modeling assumptions are given in [6]) initiates by developing CVBEM approximators [10] $\hat{\omega}_f(z)$ and $\hat{\omega}_t(z)$ for the frozen and thawed domains, respectively. The numerical technique determines the analytic function $\hat{\omega}(z)$ that satisfies the boundary conditions of either normal flux or temperature specified at nodal points located on the problem boundary Γ. Because $\hat{\omega}(z)$ is analytic throughout the interior domain Ω enclosed by Γ, the real and imaginary parts of $\hat{\phi}(z) + i\hat{\psi}(z)$ both exactly satisfy the Laplace equation over Ω.

For the steady-state condition, the governing heat flow equations reduce to the Laplace equations. Consequently, an $\hat{\omega}(z)$ determined for both the frozen and thawed regions satisfies the Laplace equations exactly, leaving only errors in satisfying the boundary conditions. To develop a CVBEM steady-state solution, an $\hat{\omega}(z)$ is developed for each of the separate regions. Initially, $\hat{\omega}_f(z)$ and $\hat{\omega}_t(z)$ are defined by

$$\begin{aligned} \hat{\omega}_f(z) &= \hat{\omega}_f^1 \qquad z \in \Omega \\ \hat{\omega}_t(z) &= \hat{\omega}_t^1 \qquad z \in \Omega \end{aligned} \tag{16}$$

where $\Omega = \Omega_t \cup \Omega_f$ is the global domain, and the first-order CVBEM approximators are based on the entire domain. This procedure results in simply estimating the 0°C isotherm location for the homogeneous problem of Ω being entirely frozen or thawed. Let C^1 be the contour corresponding to this 0°C isotherm.

The second iteration step begins by defining Ω_f^2 and Ω_t^2 based on the mutual boundary of C^1. CVBEM approximators $\hat{\omega}_f^2$ and $\hat{\omega}_t^2$ are then defined for Ω_f^2 and Ω_t^2, respectively.

Examining the stream functions $\hat{\psi}_f^2$ and $\hat{\psi}_t^2$, estimates of the discrepancy in matching the flux rates along the interface between Ω_t and Ω_f can be evaluated. The

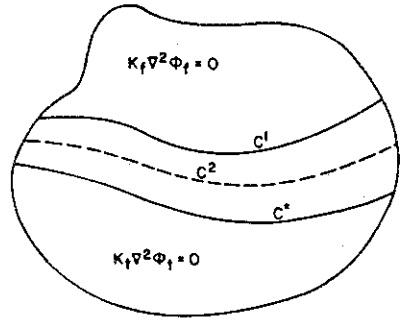

Fig. 2 Iterative estimation of freezing front location.

$\hat{\omega}_f^2$ function is now used to determine the next location of the 0°C isotherm. This is accomplished by determining a new $\hat{\omega}_f^*$ with the stream function values of $\hat{\omega}_f^2$ (modified by conductivity) superimposed at the nodal values of C^1. Next, a new 0°C isotherm C^* is located for $\hat{\omega}_f^*$. The next estimated location for the 0°C isotherm, C^2, is located by averaging the y coordinates of the nodal points between C^1 and C^*. Figure 2 illustrates this procedure. The third iteration step proceeds by defining Ω_f^2 and Ω_t^2 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

$$\left| k_f \frac{d\hat{\psi}_f}{ds} - k_t \frac{d\hat{\psi}_t}{ds} \right| < \epsilon \qquad z \in C \tag{17}$$

Using the Approximate Boundary

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 $\hat{\omega}_f$ and $\hat{\omega}_t$ that satisfy the Laplace equation over Ω_f and Ω_t, respectively. Consequently, the only approximation error occurs in matching the boundary conditions continuously on Γ_f, Γ_t, and C. The generalized Fourier series develops the best CVBEM approximation that minimizes the norm in Eq. (14), where, because of the use of analytic functions as basis functions,

$$(\phi,\phi) = \int_\Gamma \phi^2 \, d\Gamma \tag{18}$$

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., $\hat{\omega}_f$,$\hat{\omega}_t$) that correspond to the boundary conditions of the problem.

For example, in Ω_f the thermal boundary conditions for a roadway embankment (Fig. 3) are defined on the problem boundary Γ_f by

$$\phi = -10°\text{C} \qquad z \in \text{top surface}$$

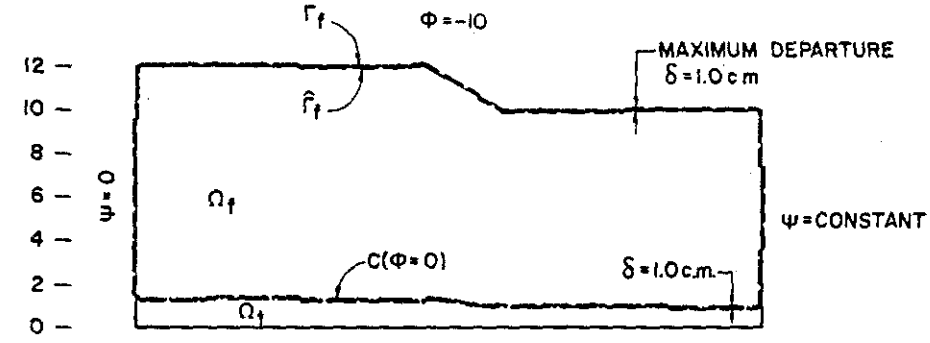

Fig. 3 Approximate boundary $\hat{\Gamma}_f$ and closeness of fit to the problem boundary Γ_f.

$$\phi = 0°C \qquad z \in \text{freezing front}$$

$$\psi = 0 \qquad z \in \text{left side (symmetry)}$$

$$\psi = \text{constant} \qquad z \in \text{right side (zero flux)}$$

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. Figure 3 also includes $\hat{\Gamma}_f$ superimposed on Γ_f. Because $\hat{\omega}_f$ is analytic within the area enclosed by 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 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 also, and 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 $\hat{\omega}_t$ equate thermal flux continuously along C.

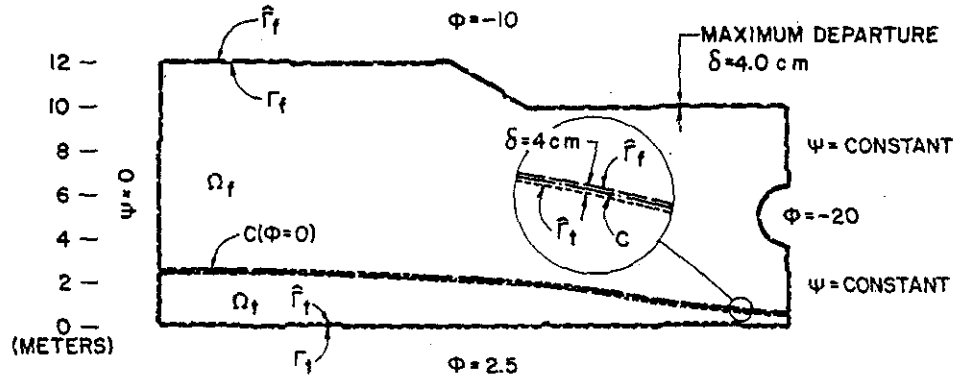

Fig. 4 Application of the CVBEM geothermal model to predict steady-state conditions.

Applications

Figure 3 depicts an application of the geothermal model for a roadway embankment problem and the use of the approximate boundary. Figure 4 illustrates the two-dimensional steady-state freezing front location on a geothermal problem involving a buried subfreezing 3-m-diameter pipeline. Examination of the approximate boundaries indicates 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

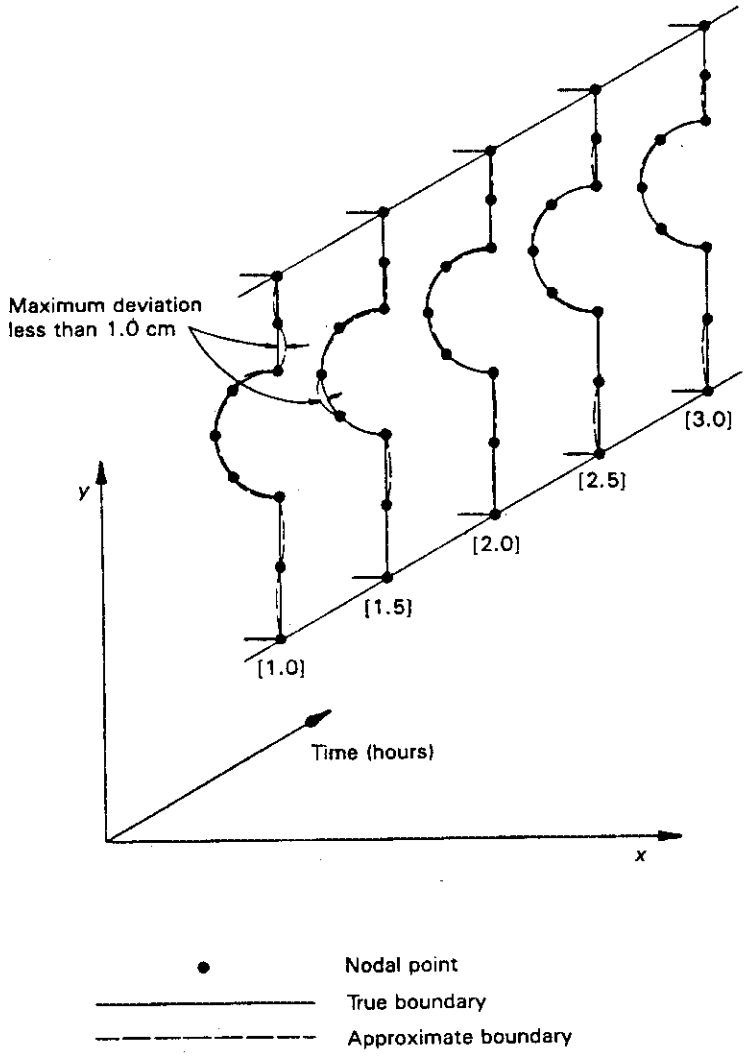

Fig. 5 Evolution of approximate boundary for time-stepped problem solution (see Fig. 3 for domain definition). (●) Nodal point; (———) true boundary; (– – –) approximate boundary.

had a value of approximately 3.5 cm. The average departure δ is estimated as less than 1 cm. The freezing front maximum departure is approximately 4 cm and occurred at the problem's 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 in estimating the freezing front is to use a finite-element or finite-difference numerical analog. A hybrid of these domain methods includes a variable mesh to better accommodate the interface. However, none of these methods provides the error of approximation. In comparison, the CVBEM model provides the approximation error not only in matching the boundary conditions but also in predicting the interface location between Ω_f and Ω_t. And this error is simple to interpret 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 the approximation error is readily seen. Figure 5 demonstrates the CVBEM modeling error in the time sequence of approximations developed for the pipe solution isolated from the problem in Fig. 4. From Fig. 5 it is concluded that the computational effort used in the CVBEM analysis is adequate for this case study. Figure 5 shows a variation in the approximate boundary location as the solution progresses in time; however, the variation is less than 1.0 cm in magnitude.

CONCLUSIONS

In this paper the CVBEM basis functions are employed in a generalized Fourier series in which the inner product of Eq. (14) is used to determine the basis function coefficients. Because analytic functions are used, the inner product reduces to a least-squares fit of the boundary conditions. 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 demonstrates the CVBEM modeling error in achieving the prescribed boundary conditions as the stepped advance in time is approximated.

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