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TECHNICAL NOTE

A NOTE ON APPROXIMATION OF ONE-DIMENSIONAL HEAT TRANSFER WITH AND WITHOUT PHASE CHANGE

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A numerical model is developed for the one-dimensional heat transfer equation with and without phase change. The numerical model is based on the nodal dimain integration method, which can represent the well-known integrated finite-difference method, the subdomain integration and Galerkin weighted residual methods, and an infinity of other finite-element lumped-mass models by the single numerical analog. A variable-order polynomial trial function is used to approximate the temperature within each finite element. Accurate solutions were obtained for the test problems considered, and the computer model requirements are small, allowing the numerical model to be accommodated with a hand-held programmable calculator.

INTRODUCTION

The technique of solving partial differential equations (PDEs) by numerical approximation is becoming increasingly attractive with the greater availability of digital computers such as current mini- and microcomputers. For some specialized problems, numerical approximation is feasible for even hand-held programmable calculators.

In this paper a numerical model of the well-known one-dimensional parabolic PDE that mathematically describes heat transfer is developed. The governing PDE is assumed to be expressed by

$$\frac{\partial}{\partial x}\left(K\frac{\partial \phi}{\partial x}\right) - C\frac{\partial \phi}{\partial t} = 0 \qquad x \in \Omega \tag{1}$$

where ϕ is the dependent variable, temperature; x and t are space and time; and K and C are the thermal conduction and capacitance terms, respectively, both assumed constant in global domain Ω. A sophisticated version of Eq. (1) including isothermal phase change of soil moisture in a freezing soil is also considered in this paper.

A review of the literature showing the current trends in numerical approximation of moisture phase change problems, such as the well-known Stefan problem, is contained in Lynch and O'Neill [1] and will not be repeated here. Usually, either the Galerkin finite-element method or an integrated finite-difference method is used to numerically solve the governing PDE. In other papers, soil moisture and heat transport models based on the control volume or subdomain integration method have been found to produce

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more accurate results than the Galerkin finite-element method (Hromadka and Guymon [2], Narasimhan and Witherspoon [3], Narasimhan et al. [4], Baliga and Patankar [5]). Hromadka and Guymon [2] examine the various numerical approaches and conclude that for problems where analytical solutions exist, the approximation error is not minimized by any of these approaches. In fact, they show that to minimize the approximation error, the method of numerical solution must change as the simulation progresses in modeled time.

Using the nodal domain integration method, Hromadka and Guymon [2] develop a finite-element matrix system that can represent the Galerkin, subdomain integration, and integrated finite-difference methods by the specification of a single mass weighting factor. For a linear trial function estimate within each finite element, the resulting element matrix systems for each of the above numerical approaches are identical except for a variation in mass weighting of the element capacitance matrix. Consequently, a unifying numerical analog is easily developed and is expressed by

$$\mathbf{A}^e(\eta) = \mathbf{S}^e\phi^e + \mathbf{P}^e(\eta)\dot{\phi}^e \tag{2}$$

where $\mathbf{A}^e$ is the finite-element matrix system for the approximation of Eq. (1) in local element Ω^e; ϕ^e and $\dot{\phi}^e$ are the element nodal state variable values and time derivative of nodal state variable values; and $\mathbf{S}^e$ and $\mathbf{P}^e(\eta)$ are element matrices defined by

$$\mathbf{S}^e \equiv \frac{K}{l^e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{3}$$

$$\mathbf{P}^e(\eta) = \frac{Cl^e}{2(\eta+1)}\begin{bmatrix} \eta & 1 \\ 1 & \eta \end{bmatrix} \tag{4}$$

where l^e is the length of element Ω^e and η is a mass weighting factor. From Eq. (2), the Galerkin, subdomain integration, and integrated finite-difference methods are given by $\eta = (2, 3, \infty)$, respectively.

Thus it is seen that from Eq. (2) an infinite of mass weighting models exist. However, no single mass weighting model (including Galerkin, finite difference, and subdomain integration) provides the best numerical approximation. The optimum definition of η that minimizes the approximation error is a function of time, such that

$$A^e(\eta) = A^e[\eta(t)] \tag{5}$$

In this paper a modification of the unifying nodal domain integration model of Eq. (2) is used to numerically approximate the two-phase Stefan problem as defined for a freezing soil. The definition of the model mass weighting factor is given by the integration of a variable-order polynomial trial function within each finite element. Because the proposed trial function family can approximate both smooth and steep function surfaces, the number of necessary finite elements is reduced, and this significantly reduces computer memory requirements.

GOVERNING EQUATIONS

A two-phase Stefan moving-boundary problem in a freezing soil is defined by

$$C_1 \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} K_1 \frac{\partial T}{\partial x} \quad \text{in } R_1 \qquad C_2 \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} K_2 \frac{\partial T}{\partial x} \quad \text{in } R_2 \tag{6}$$

where C_1 and K_1 are the volumetric heat capacity and thermal conductivity of frozen soil and C_2 and K_2 are the appropriate unfrozen thermal parameters. The problem domain of definition is divided into the regions R_1 and R_2 by a moving boundary S, defined by

$$L \frac{dS}{dt} = K_1 \frac{\partial T}{\partial x}\bigg|_{S^-} - K_2 \frac{\partial T}{\partial x}\bigg|_{S^+} \tag{7}$$

where L is the volumetric latent heat of fusion of the soil water available for freezing.

The one-dimensional freezing soil problem is further defined by the boundary conditions of a freezing and subfreezing temperature imposed on respective ends of the problem domain, with the initial condition of the soil-water mixture being specified at a thawed temperature.

Without phase change, the governing heat equations can be reduced to the well-known normalized problem with conditions

$$\begin{aligned} \xi(t=0) &= 1 \qquad 0 \leqslant x \leqslant 1 \\ \xi(x=0, t>0) &= \xi(x=1, t>0) = 0 \end{aligned} \tag{8}$$

where ξ is a normalized variable substitution for the dependent variable temperature, and the problem domain of definition is redefined as $\{x : 0 \leqslant x \leqslant 1\}$.

Both heat transfer problems described above will be modeled by the numerical methods presented in the following sections. For the normalized heat transfer problem with conditions of Eq. (8), symmetry is used to redefine the problem with a zero-flux (Neumann) boundary condition at the midpoint of the domain, and then one finite element is used to approximate the temperature profiles as the solution progresses in time. For the two-phase Stefan problem, specified boundary temperatures (Dirichlet) at the endpoints of the problem and at the freezing front are used as follows:

$$\left.\begin{aligned} T &= T_F \quad x = 0 \\ T &= T_U \quad x = \infty \quad T_F < 0^\circ\text{C} < T_U \\ T &= T_U \quad t = 0 \end{aligned}\right\} \tag{9}$$

where the freezing point temperature is 0°C. For the phase change problem, two finite elements are used with nodal points defined at the freezing front and at $x = \{0, x_0\}$, where x_0 is arbitrarily large to approximate the second condition stated in Eq. (9).

The trial functions $\hat{\phi}^e$ to be used in each local finite element Ω^e are the two families defined on ϕ^e by

$$\hat{\phi}^e \equiv \begin{cases} N_1 \phi_1^e + N_2 \phi_2^e & \dfrac{\partial \hat{\phi}^e}{\partial t} \leqslant 0 \\ M_1 \phi_1^e + M_2 \phi_2^e & \dfrac{\partial \hat{\phi}^e}{\partial t} \geqslant 0 \end{cases} \tag{10}$$

where the $\{N_i, M_i\}$ trial function family depends on whether there is accumulation of heat within the finite element Ω^e and the subscripts denote a concave-down or concave-up function. The definitions of $\{N_i, M_i\}$ used are

$$[N_1, N_2] \equiv [(1 - \hat{y}^n), \hat{y}^n] \tag{11}$$

$$[M_1, M_2] = [(1 - \hat{y})^n, 1 - (1 - \hat{y})^n] \tag{12}$$

where $\hat{y}$ is a finite-element local coordinate for a two-endpoint-node element with nodes at $\hat{y} = (0, 1)$. The order n of the shape functions is determined by the numerical model as part of the problem solution. Consequently, knowledge of the nodal values and the order of the trial function polynomial gives a significantly better estimate of the solution interior to each finite element than is obtained by the linear trial functions often used.

NUMERICAL METHOD

The local element matrix systems for finite element Ω^e are given by

$$\mathbf{S}^e \phi^e \equiv \begin{Bmatrix} \left(K \dfrac{\partial \phi}{\partial x}\right)\Big|_{Z_e} \\ * \\ * \\ \left(K \dfrac{\partial \phi}{\partial x}\right)\Big|_{Z_e} \end{Bmatrix} \qquad \mathbf{P}^e \equiv \begin{bmatrix} \displaystyle\int_0^{Z_e} N_1 \, d\hat{y} & \displaystyle\int_0^{Z_e} N_2 \, d\hat{y} \\ \displaystyle\int_{Z_e}^0 N_1 \, d\hat{y} & \displaystyle\int_{Z_e}^0 N_2 \, d\hat{y} \end{bmatrix} \tag{13}$$

where * indicates the evaluation of flux at finite-element boundaries and Z_e is chosen such that $\mathbf{P}^e$ is symmetric. That is,

$$\int_0^{Z_e} N_2 \, d\hat{y} \equiv \int_{Z_e}^1 N_1 \, d\hat{y}$$

defines Z_e for each local finite element Ω^e.

From Eq. (13),

$$Z_e = \frac{n}{n+1} : N_i \text{ family} \qquad Z_e = \frac{1}{n+1} : M_i \text{ family} \tag{14}$$

where n is the order of the N_i shape function family. For the N_i trial functions the variable lumped-mass capacitance matrix is given by

$$\mathbf{P}^e = \frac{Cl^e}{n+1}\begin{bmatrix}(n-\alpha) & \alpha \\ \alpha & (1-\alpha)\end{bmatrix} \qquad \alpha = Z_e^{n+1} \tag{15}$$

The conduction matrix is also a function of time and is given by

$$\mathbf{S}^e = \frac{Kn(n/n+1)^{n-1}}{l^e}\begin{bmatrix}1 & -1 \\ -1 & 1\end{bmatrix} \tag{16}$$

where for nonlinear problems K is the thermal conductivity evaluated at $\hat{y} = Z_e$.

Examination of the local element matrix systems indicates that a time-dependent lumped-mass scheme has been developed in which the element conduction and capacitance matrices change as the solution progresses in time. The element matrix variability, however, needs to be defined so that the matrices can be developed. Initially, the order of the trial function is specified based on knowledge of the initial conditions of the problem.

For modeling purposes, an explicit finite-difference approximation is used to approximate

$$\left(\frac{\partial}{\partial x}K\frac{\partial \phi}{\partial x} - C\frac{\partial \phi}{\partial t}\right)\bigg|_{Z_e} = 0 \tag{17}$$

where for the normalized heat transfer problem, Eq. (17) is approximated with

$$\left(\frac{\phi^{i+1} - \phi^i}{\Delta t}\right)\bigg|_{Z_e} = \left(\frac{\partial^2 \hat{\phi}^e}{\partial x^2}\right)\bigg|_{Z_e} \tag{18}$$

where the superscripts are time step notation. In Eq. (18), $\hat{\phi}^e$ is the trial function in local element Ω^e, and the second derivative is evaluated based on the most recent assumed order of the trial function. From Eq. (18),

$$\phi^{i+1}(Z_e) = \phi^i(Z_e) + \Delta t\left(\frac{\partial^2 \hat{\phi}^e}{\partial x^2}\right)\bigg|_{Z_e} \tag{19}$$

where Δt is the time step size, which is also determined as part of the problem solution.

To evaluate the time step, the model assumes the usual explicit method stability criteria; i.e.,

$$\frac{\Delta t}{(\Delta x)^2} \leqslant \frac{1}{2} \qquad \Delta x = \min\left[l^e(1-Z_e), l^e Z_e\right] \tag{20}$$

From Eqs. (19) and (20), $\phi^{i+1}(Z_e)$ is approximated. From Eq. (2), the nodal values ϕ^e are approximated. Updated values of the trial function order n are determined by passing a trial function through the new ϕ^e values and $\phi^{i+1}(Z_e)$ for each successive time step advancement.

MODEL APPLICATIONS

Problems of heat transfer with and without soil water phase change in a freezing soil were numerically modeled by the proposed methods. To begin the model solution, an initial condition is defined to closely approximate the actual initial conditions of the problem. For example, a polynomial trial function of arbitrarily high order ($n = 100$) was used for the initial trial function approximation of temperature in the finite element for the heat transfer problem without phase change. The well-known Crank-Nicolson time advancement method is used to solve for the time derivative of temperature. The model determines the time advancement time step size Δt, subsequent trial function polynomial orders n, and mass-lumped matrix symmetry local coordinates Z_e as part of the model solution according to the equations given above.

Because of the simple computer coding and minimal requirements for model variable storage, both test problems were numerically approximated with a programmable hand-held calculator. A Texas Instruments 58A calculator was used in this study, but other programmable calculators are equally suitable for problems of this level of complexity.

Figure 1 shows computed normalized temperature profiles at various unit time levels along with the analytical solution profiles for the normalized heat transfer problem without phase change. Approximation profiles were plotted by using the single (midpoint) nodal temperature values from the finite-element model and incorporating the approximated polynomial trial function. Figure 2 shows the modeled parameter variations of n, Z_e, and Δt plotted against the model time step number. From Fig. 2, the initially high-order polynomial trial function model utilizes a small time step size. As the solution progresses in time, the polynomial order approaches the limiting value $n = 1.66$; the model time step Δt and other model parameters also approach limiting values, as shown in Fig. 2.

For the two-phase Stefan problem, Fig. 3 shows modeled and analytical values of

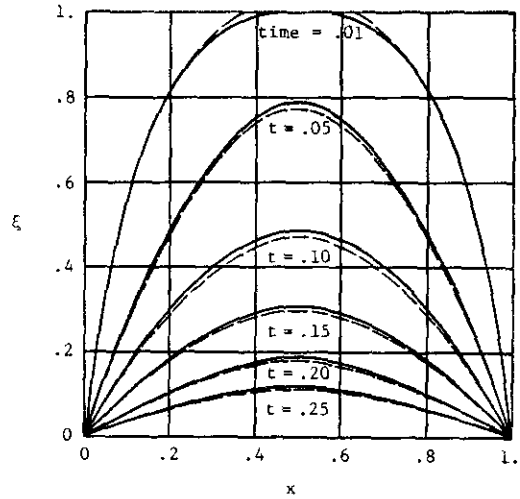

Fig. 1 Analytical solution (dashed line) and approximation results (solid line) for normalized heat transfer problem with a one-finite-element model.

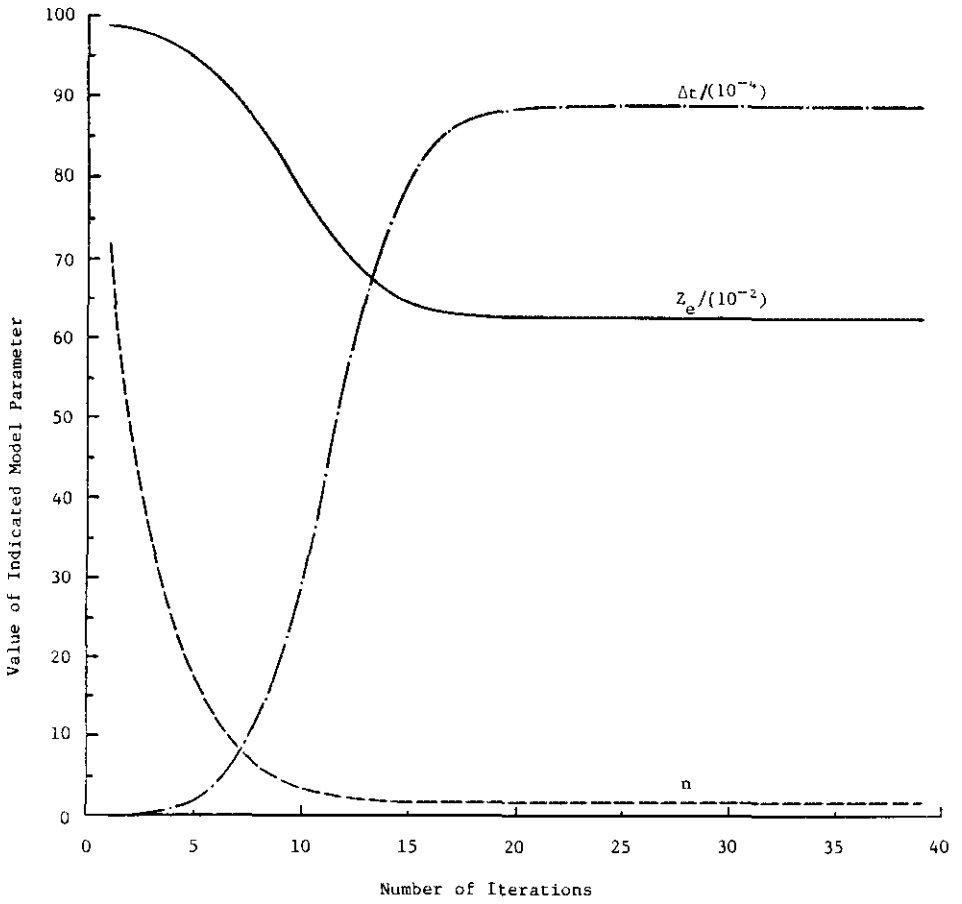

Fig. 2 Plot of model variables Δt, Z_e, and trial function order n in approximation of normalized heat transfer problem.

the freezing front penetration into a soil column. Values of 0.62 cal/cm^3 for C, 9.6 X 10^{-3} cal/cm·s·°C^{-1} for K, and 17.68 cal (per cubic centimeter of soil) for L were used, which are appropriate for a water-saturated, dense sand. The same problem was considered by Lynch and O'Neill [1]. Figure 3 shows that good agreement is obtained in the prediction of freezing front penetration when the two-element numerical model is used. Only the initial portion of the numerical model results is shown in Fig. 3 because of the continued close agreement between approximated and analytical results. The results from the proposed model closely match the numerical modeling results from Lynch and O'Neill, who used a computationally more elaborate method based on a Galerkin finite-element convection-diffusion type of model with a deforming one-dimensional grid approximation, which also required 10 Hermitian cubic elements in the finite-element model.

CONCLUSIONS

A new efficient numerical method has been employed with the classical two-phase Stefan problem. The proposed method is based on the nodal domain integration (variable

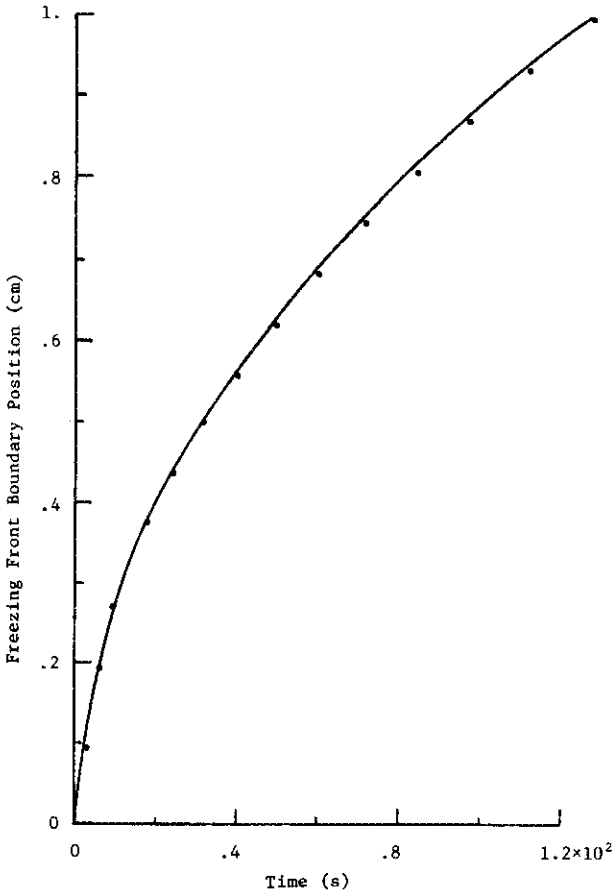

Fig. 3 Analytic solution (solid line) and approximation results (points) in model of two-phase Stefan problem.

lumped-mass finite-element) method, and incorporates a sophisticated variable-order polynomial trial function within each finite element. Some advantages of this family of "smart" trial functions are as follows:

1. Reduces the need for fine discretization of the one-dimensional domain near the freezing front.
2. Reduces the need to use a moving-boundary variable finite-element mesh.
3. Reduces the number of finite elements needed to produce similar levels of approximation accuracy.
4. Provides supplemental trial function information, which can be used to accurately analyze the function surface within large finite elements.
5. Models a sharp function surface or interface with a minimum of finite elements.

Although the test problems presented in this paper are simple, an extension to more general one-dimensional problems should result in more efficient codes, especially for problems that involve interface or sharp function surfaces in the solution. Extension of the method to multidimensional problems is not obvious and requires further research.

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