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EFFICIENT NUMERICAL TECHNIQUE FOR ONE-DIMENSIONAL THERMAL PROBLEMS WITH PHASE CHANGE

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Abstract—A new numerical scheme for one-dimensional heat flow problems with phase change is presented. The technique, which continuously monitors the progression of the phase interface, is unusual for the high accuracy achieved without sacrifice to computing efficiency.

NOMENCLATURE

- C, heat capacity per unit volume;
- CN, thermal conductance coefficient, Fig. 1;
- E, E', Gaussian elimination coefficients, equations (7a), (9a);
- G, H, position of moving phase change interface;
- HC, heat capacity coefficient, Fig. 1;
- k, thermal conductivity;
- L_v, latent heat per unit volume;
- S, S', Gaussian elimination coefficients, equations (7b), (9b);
- T, temperature;
- t, time;
- x, depth.

Greek symbols

- Δt, time step;
- Δx, space interval;
- ΔT, temperature range;
- θ, unfrozen moisture (volume basis).

Subscripts

- A, apparent;
- f, frozen or freezing;
- i, node index;
- m, time step index;
- N, node index for fixed boundary;
- p, node index for element undergoing phase change;
- u, thawed or unfrozen.

FOR DESIGNING roadways and other engineering works in cold climates, as well as for more fundamental studies of ground temperature regimes in nature, it is useful and often essential to have available numerical techniques for calculating the depth of frost or thaw penetration. For long-term computations involving many annual cycles, high numerical efficiency is required in order to minimize costs. Road embankment calculations are usually concerned with layered systems composed of materials that possess a narrow freezing range. The most appropriate techniques for such cases are those that locate directly the position of the moving freezing or thawing interface. Because of certain numerical difficulties, these methods have not found favour in the past. The method now presented circumvents such difficulties and yields accurate solutions at low cost for these and other similar moving interface problems.

EXISTING METHODS

One-dimensional freezing or thawing with latent heat release (+) or absorption (−) at a fixed temperature is described by the conditions

$$k_f \left.\frac{\partial T}{\partial x}\right|_z - k_u \left.\frac{\partial T}{\partial x}\right|_z = (\pm) L_v \frac{\mathrm{d}z}{\mathrm{d}t} \tag{1}$$

and

$$T(z,t) = T_f = \text{constant} \tag{2}$$

at the moving interface. The heat conduction equation

$$\frac{\partial}{\partial t}(C \cdot T) = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) \tag{3}$$

applies in the frozen and unfrozen regions on either side of the moving phase boundary, due account being taken of differences in thermal properties.

Numerical treatments of phase change generally replace the moving boundary condition [equation (1)] by a latent heat source term added to the heat conduction equation to yield an apparent heat capacity formulation

$$\frac{\partial}{\partial t}(C_A T) = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) \tag{4}$$

with

$$C_A = C_t \quad \text{for} \quad T > T_f \tag{4a}$$

and

$$C_A = C_f + L_v \partial\theta/\partial T \quad \text{for} \quad T < T_f \tag{4b}$$

where

$\theta = \theta(T, x) =$ unfrozen volumetric moisture content.

In practice, the entire latent heat is usually associated with a small finite temperature range ΔT and equation

(4b) is replaced by

$$C_A = C_f + L_v/\Delta T \quad \text{for} \quad T_f - \Delta T < T < T_f$$
$$C_A = C_f \quad \text{for} \quad T < T_f - \Delta T.$$

Although apparent heat capacity formulations have the advantage of being simple to programme, the predicted phase change interface location, corresponding to the isotherm $T = T_f$, advances in an unphysical oscillatory fashion and this is accompanied by distortion of the temperature profile in the region undergoing phase change. In order to hold errors within acceptable bounds the grid spacing in that region may have to be reduced substantially. This can, however, result in a situation in which the T_f-isotherm moves across a grid element in less than one time step and the element latent heat contribution can be missed entirely unless the time step also is reduced. Spatial resolution of the phase change interface location is poor, and this can be critical when dealing with layered problems with sharp contrast in thermal properties between neighbouring layers such as insulated road embankments. Inability to accommodate two phase change planes existing simultaneously within the same grid element can lead to errors in certain periodic thermal regime problems where coalescence is important. As well, in time-dependent boundary condition problems the error associated with oscillation can be cumulative. These difficulties are exacerbated when dealing with materials that possess a narrow freezing range or freeze at fixed temperature. Several different apparent heat capacity formulations have already been described [1–6].

Only a limited number of formulations have been given that incorporate equation (1). Douglas and Gallie [7] and Kazemi and Perkins [8] describe methods that use variable time steps whose length must be found by nodal iteration, though the formulation uses explicit time differencing. A time dependent grid spacing scheme, also requiring nodal iteration, has been proposed by Heitz and Westwater [9] and Murray and Landis [10]. Both methods are restricted to homogeneous media and are not suited to practical calculations.

It is also possible, and certainly preferable, to solve the system defined by equations (1)–(3) for the local position of the phase change plane within an element of fixed dimensions using fixed time steps. Crank [11] and Ehrlich [12] used higher order space differences for the phase change interface equation and this restricts the method to homogeneous media, at the same time necessitating intricate programming in order to move the interface across element boundaries. The formulation of Meyer *et al.* [13] is a lumped-parameter scheme using finite differences for the time dimension only. It is flexible, but a considerable amount of computation is required at each time step. Hwang [14] presented a scheme in which an equivalent of equation (1) can be used to estimate an elemental latent heat source term for inclusion in a two-dimensional finite-element formulation. The latent heat is considered to be distributed over the element in a manner similar to that of apparent heat capacity formulations, and the phase change interface location is not followed continuously as such. The initial T_f-isotherm position is, instead, estimated at each time step by linear interpolation of the corresponding temperature profile. In addition, the non-linearity associated with the phase change equation and hence the necessity of using nodal iteration for solution is eliminated by using a forward difference approximation for the latent heat contribution. Although these approximations can be justified on practical grounds for two-dimensional problems, the resulting numerical accuracy is not so high as could otherwise be achieved.

Many of the drawbacks associated with these methods can be circumvented, and it is the purpose of this paper to describe a technique capable of locating the phase change interface in one-dimensional layered systems accurately and efficiently. The method uses a centred-difference formulation with solution by simple Gaussian elimination at ordinary nodes. The element undergoing phase change is treated by a technique that continuously follows the position of the moving phase change interface by means of a formulation that maintains the non-linear character of the problem without requiring costly nodal iterations for solution.

PROPOSED NUMERICAL TECHNIQUE FOR PHASE CHANGE AT FIXED TEMPERATURE

The centred time difference equation for layered systems can be written

$$HC_i \cdot (T_i^{m+1} - T_i^m) = CN_{i-1} \cdot (T_{i-1}^{m+1} - T_i^{m+1} + T_{i-1}^m - T_i^m) + CN_i \cdot (T_{i+1}^{m+1} - T_i^{m+1} + T_{i+1}^m - T_i^m) \quad (5)$$

where i and m are space and time indices, respectively. The heat capacity coefficients HC and conductance coefficients CN are defined in Fig. 1. Rearranging, the equation may be cast in the form

$$-CN_{i-1} \cdot T_{i-1}^{m+1} + (HC_i + CN_{i-1} + CN_i) \cdot T_i^{m+1} - CN_i \cdot T_{i+1}^{m+1} = \mathrm{RHS}_i \quad (6)$$

where

$$\mathrm{RHS}_i = CN_{i-1} \cdot T_{i-1}^m + (HC_i - CN_{i-1} - CN_i) \cdot T_i^m + CN_i \cdot T_{i+1}^m.$$

With boundary temperatures prescribed at nodes $i = 0$ and $i = N$ corresponding to the upper and lower surfaces, respectively, the unknown temperatures T_i^{m+1}, $1 < i < N-1$ can be found by solving the system of equations represented by equation (6) using Gaussian elimination. Two equivalent formulations are possible. Upper triangulation (forward elimination) yields

$$E_0 = T_0^{m+1} \text{ (prescribed)}$$
$$S_0 = 0$$
$$E_i = (\mathrm{RHS}_i + CN_{i-1} \cdot E_{i-1})/D \quad (7a)$$
$$S_i = CN_i/D \quad (7b)$$

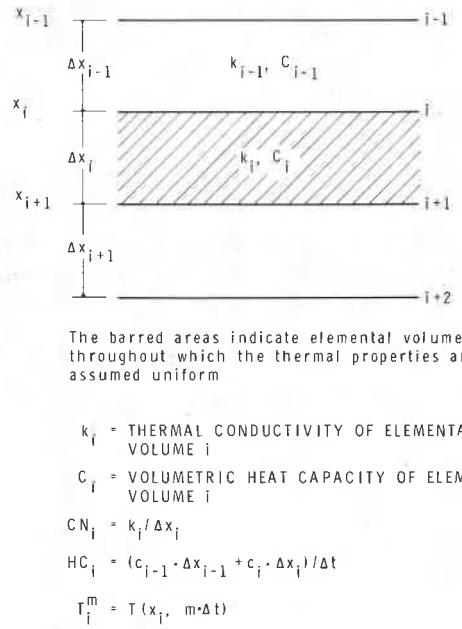

FIG. 1. Definition of finite difference grid used for inhomogeneous materials.

where

$$D = HC_i + CN_{i-1} + CN_i - CN_{i-1} \cdot S_{i-1}$$

and

$$i = 1 \quad \text{to} \quad N-1.$$

After successive evaluation of the coefficients E_i, S_i, the nodal temperatures may be determined from the backward substitution equation

$$T_i^{m+1} = S_i \cdot T_{i+1}^{m+1} + E_i \tag{8}$$

where

$$i = N-1 \quad \text{to} \quad 1$$

and

T_N^{m+1} is prescribed.

For lower triangulation (backward elimination)

$$E'_N = T_N^{m+1} \text{ (prescribed)}$$

$$S'_N = 0$$

$$E'_i = (\text{RHS}_i + CN_i \cdot E_{i+1})/D \tag{9a}$$

$$S'_i = CN_{i-1}/D \tag{9b}$$

where

$$D' = HC_i + CN_{i-1} + CN_i - CN_i \cdot S_{i+1}$$

and

$$i = N-1 \quad \text{to} \quad 1.$$

The unknown nodal temperatures are successively determined from the forward substitution equation

$$T_i^{m+1} = S'_i \cdot T_{i-1}^{m+1} + E'_i \tag{10}$$

where

$$i = 1 \quad \text{to} \quad N-1$$

and

T_0^{m+1} is prescribed.

If a moving phase boundary is present within an elemental volume bounded by nodes p and $p+1$, the element can be split into two zones as shown in Fig. 2. Zones a and b have thermal properties C_a, k_a and

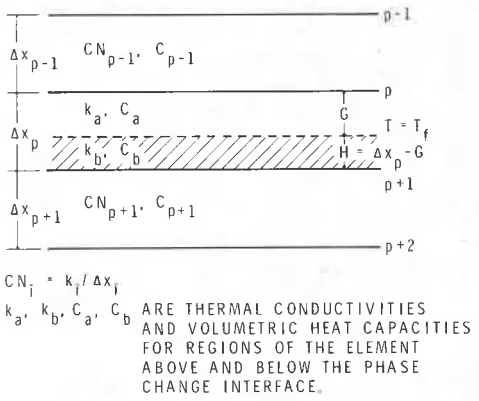

FIG. 2. Definition of finite difference grid used for phase boundary treatment.

C_b, k_b, respectively. Using central differences and assuming $T_f = 0$ for convenience, heat balance for node $i = p$ yields

$$\tfrac{1}{2}(C_{p-1} \cdot \Delta x_{p-1} + C_a \cdot \bar{G}) \cdot (T_p^{m+1} - T_p^m)/\Delta t = \tfrac{1}{2} CN_{p-1} \cdot (T_{p-1}^{m+1} - T_p^{m+1} + T_{p-1}^m - T_p^m) - \tfrac{1}{2} \frac{k_a}{\bar{G}} \cdot (T_p^{m+1} + T_p^m) \tag{11}$$

where $\bar{G} = \tfrac{1}{2}(G^{m+1} + G^m)$, and $G^m(G^{m+1})$ is the distance below x_i of the T_f-isotherm at the beginning (end) of the time step. At node $p+1$,

$$\tfrac{1}{2}(C_{p+1} \cdot \Delta x_{p+1} + C_b \cdot \bar{H}) \cdot (T_{p+1}^{m+1} - T_{p+1}^m)/\Delta t = \tfrac{1}{2} CN_{p+1} \cdot (T_{p+2}^{m+1} - T_{p+1}^{m+1} + T_{p+2}^m - T_{p+1}^m) - \tfrac{1}{2} \frac{k_b}{\bar{H}} \cdot (T_{p+1}^{m+1} + T_{p+1}^{m+1}) \tag{12}$$

where

$$\bar{H} = \Delta x_p - \bar{G}.$$

The moving boundary condition, equation (1), is approximated by the central difference equation

$$\pm L_v(G^{m+1} - G^m)/\Delta t + \tfrac{1}{2}\{\tfrac{1}{2} C_a (T_{p-1}^{m+1} + T_{p-1}^m) - \tfrac{1}{2} C_b (T_{p+1}^{m+1} + T_{p+1}^m)\} = \tfrac{1}{2} k_a \frac{(T_p^{m+1} + T_p^m)}{\bar{G}} + \tfrac{1}{2} k_b \frac{(T_{p+1}^{m+1} + T_p^m)}{\bar{H}}. \tag{13}$$

The second term on the left of equation (13) is included to account for enthalpy change associated with the elemental specific heat capacities. It arises because the equation represents a heat balance for a region of finite dimensions. Although not essential, this additional term does improve accuracy, particularly when the latent heat is small compared with the

specific heat capacity terms. Heat transfer at the remaining ordinary nodes is described by equation (5). As G^{m+1} is not known explicitly, the system including equations (5) and (11)–(13) is non-linear. Introduction of nodal iteration can, however, be avoided by judicious use of both forward and backward Gaussian elimination.

From the forward elimination formula, equation (7), the coefficients E_i, S_i can be determined successively for $i = 1$ to $i = p-1$. For node $i = p$, equation (11) leads to

$$E_p = \frac{CN_{p-1} \cdot (T_{p-1}^m + E_{p-1}) + \left(C_{p-1} \cdot \frac{\Delta x_{p-1}}{\Delta t} + \frac{C_a \cdot \bar{G}}{\Delta t} - CN_{p-1} - \frac{k_a}{\bar{G}} \right) \cdot T_p^m}{C_{p-1} \cdot \frac{\Delta x_{p-1}}{\Delta t} + \frac{C_a \cdot \bar{G}}{\Delta t} + \frac{k_a}{\bar{G}} + CN_{p-1}(1 - S_{p-1})} \tag{14}$$

and from equation (8)

$$T_p^{m+1} = S_p \cdot T_f + E_p$$

or, since

$$T_f = 0$$

$$T_p^{m+1} = E_p, \tag{15}$$

Similarly, the backward elimination technique, equation (9) and (10), for the region below the phase plane gives

$$T_{p+1}^{m+1} = E'_{p+1} \tag{16}$$

where, following equation (12)

$$E'_{p+1} = \frac{CN_{p+1} \cdot (T_{p+2}^m + E'_{p+2}) + \left(C_{p+1} \cdot \frac{\Delta x_{p+1}}{\Delta t} + C_b \cdot \frac{\bar{H}}{\Delta t} - CN_{p+1} - \frac{k_b}{\bar{H}} \right) T_{p+1}^m}{C_{p+1} \cdot \frac{\Delta x_{p+1}}{\Delta t} + C_b \cdot \frac{\bar{H}}{\Delta t} + \frac{k_b}{\bar{H}} + CN_{p+1}(1 - S'_{p+2})} \tag{17}$$

and the coefficients E'_i, S'_i are calculated successively from equation (9) with $i = N-1$ to $i = p+2$.

It should be noted that in both equations (14) and (17) all terms on the RHS are known explicitly except G^{m+1}. The introduction of forward elimination above, and backward elimination below, the moving boundary has the effect of isolating the non-linearity associated with the moving interface. Equation (13) combined with equations (15) and (16) is a non-linear, ordinary difference equation whose solution yields G^{m+1} and the nodal temperatures T_p^{m+1} and T_{p+1}^{m+1} simultaneously. The remaining nodal temperatures can be determined from the appropriate backward or forward substitution equation, without recourse to nodal iteration. Equations (13), (15) and (16) can be solved by any convenient method. The Secant method is appropriate and converges after four or five iterations at most. Simple iteration is also satisfactory.

To complete the numerical formulation it is necessary to provide a means of permitting the phase change interface to move across an element boundary. This may be accomplished by splitting the time step.

$$\Delta t = \Delta t_1 + \Delta t_2$$

where

Δt_1 = time interval required to move the T_f-isotherm to the element boundary. Assuming velocity constant over a time step, then whenever equation (13) yields

$$G^{m+1} = G' > \Delta x_p,$$

Δt_1 can be approximated by

$$\Delta t_1 = \frac{(\Delta x_p - G^m)}{G' - G^m} \Delta t. \tag{18}$$

Nodal temperatures are updated using the partial time step Δt_1, after which displacement of the phase change plane within the neighbouring element $i = p+1$ is evaluated for the remaining interval Δt_2; the nodal temperatures are then updated to their final values T_i^{m+1}. An analogous procedure is used whenever $G' < 0$.

VERIFICATION OF THE METHOD

Figure 3 compares an analytical and two numerical solutions for a simplified Neumann freezing problem. Comparison is based on frost penetration and it may be noted that this offers a more sensitive test of the quality of the method than does the more usual comparison of temperature profiles. The following parameter values were chosen:

$$T(x,0) = T_{\text{initial}} = +2°\text{C}$$

$$T(0,t) = T_{\text{surface}} = -10°\text{C} \quad t > 0$$

$$T(\infty,t) = T_{\text{initial}} \quad t \geqq 0$$

$$k_f = k_t = 2\ \text{W/m}\cdot\text{K}$$

$$L_v = 100\ \text{MJ/m}^3.$$

Thermal conductivities and heat capacities were assumed to be identical in the frozen and thawed regions to ensure that differences in results obtained by the numerical methods were due only to the assumptions

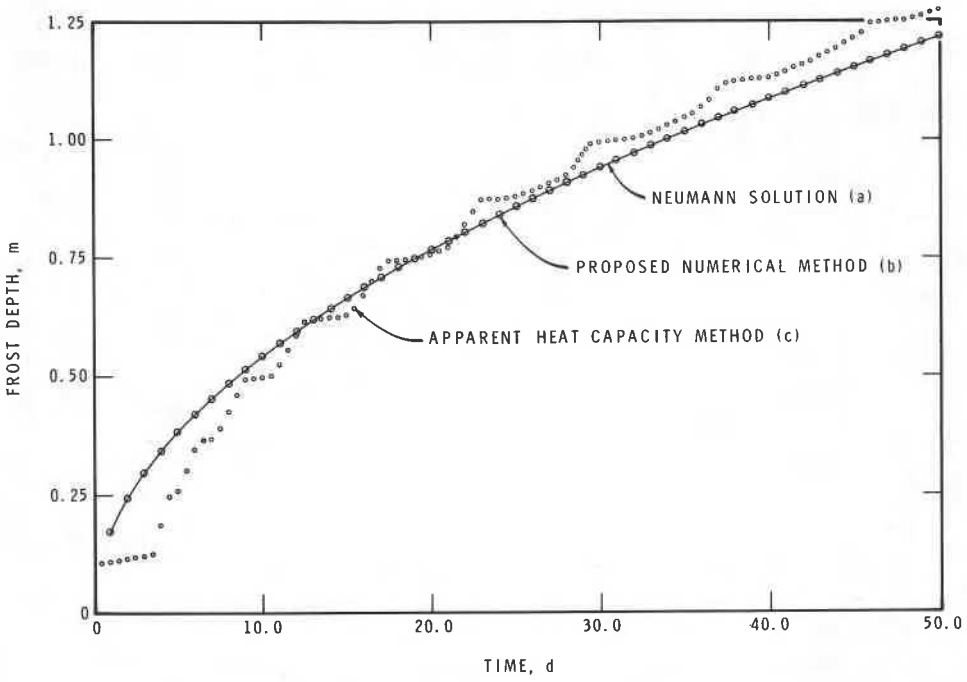

FIG. 3. Comparison of two numerical methods vs analytic solution for frost penetration.

made in the treatment of latent heat. Curve (a) shows the frost penetration calculated from the analytical solution; curve (b) was computed using the numerical method presented here. For comparison, curve (*c*) was calculated using an apparent heat capacity formulation assuming a freezing range of 0.5 K. A Crank–Nicholson formula was used with thermal properties updated at each time step. In both cases precautions were taken to eliminate the starting error associated with the step-function surface condition. Results for the author's method were calculated using a grid spacing and time step

$$\Delta x = 0.25\,\text{m}$$
$$\Delta t = 1\,\text{day}$$

while the apparent heat capacity formulation required

$$\Delta x = 0.125\,\text{m}$$
$$\Delta t = 0.25\,\text{day}.$$

This represents nearly an eight-fold increase in computation time.

It may be seen that the present method follows very closely the true frost penetration at all times, with no tendency to oscillate. Accuracy is such that results are essentially indistinguishable from those of the analytic solution. The relative crudeness of the apparent heat capacity method is evident.

A second comparison is presented in Fig. 4, in which the problem is similar to that of Fig. 3 except for the thermal properties, which were taken as

$$k_f = 2.25\,\text{W/m}\cdot\text{K}$$
$$C_f = 1.5\,\text{MJ/m}^3$$
$$k_t = 1.75\,\text{W/m}\cdot\text{K}$$
$$C_t = 2.5\,\text{MJ/m}^3.$$

Degeneration of the numerical results is minimal. Although not shown, the relative performance of the apparent heat capacity formulation would have been even worse in this case than in the previous one inasmuch as the solution oscillations are no longer compensated symmetrically.

DISCUSSION

The proposed method offers a number of advantages when compared with existing techniques. The rather exceptional accuracy inherent in the formulation is obtained with no loss of efficiency and, in fact, computation times are essentially the same as those required for the central difference calculation at the ordinary nodes. The method is completely flexible, and layered systems with sharp contrasts in thermal properties, either between layer boundaries or associated with change of phase, can be handled efficiently without degradation of solution accuracy. Because the solution accurately tracks the true frost penetration at all times, high accuracy can be maintained even in problems with rapidly changing surface boundary conditions. The latent heat formulation does not in itself impose restrictions on the size of grid spacing or time step. These are limited only by the usual truncation error associated with the Crank–Nicholson equations for the ordinary nodes.

The latent heat treatment, as described, is restricted to problems with a single freezing or thawing front. Situations involving more than one phase interface can occur, for example, in the study of annual ground thermal regimes. The combined backward and forward Gaussian elimination solution technique cannot be used to avoid nodal iteration if two phase planes are present. In many practical cases, however, temperatures in the zone between the two phase interfaces

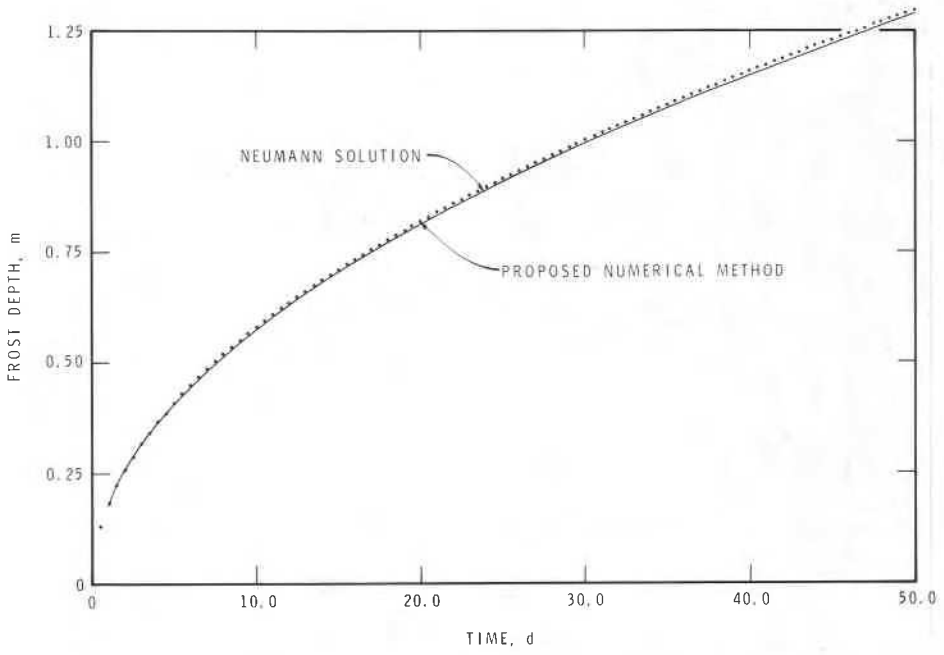

FIG. 4. Calculated frost depth comparison—non-constant thermal properties.

rapidly approach the freezing point. Under these conditions heat flow is small compared with values outside the zone and can be ignored. A single-sided formulation of the method can then be used for each phase change plane separately, and in this way nodal iteration can be avoided. In addition, coalescence of the phase change planes can be followed even when both interfaces occur within the same element. This approach was used in a programme developed to study the effects of snow cover on ground thermal regimes. Complete FORTRAN programmes based on earlier versions of the formulation have been given [15–17]. If nodal iteration cannot be tolerated for problems with multiple phase interfaces, where the isothermal assumption cannot be made or where thermal properties are very strong functions of temperature, it may be desirable to reformulate the method using a three time level scheme. This approach is to be considered in a future study.

CONCLUSION

A new numerical technique for treating one-dimensional problems with phase change has been developed. The numerical accuracy of the method is much superior to that of the apparent heat capacity formulation. The solution technique retains the non-linearity associated with the moving phase boundary without requiring costly nodal iteration. The resulting high efficiency is further enhanced by the insensitivity of the method to size of grid spacing and time step.

Comparison with the analytical solution for a simplified problem showed that the numerical method yields results closely following those for analytically calculated frost penetration. In contrast with the apparent heat capacity formulation, the solution showed no tendency to oscillate and the high accuracy achieved was maintained at all times. Comparison with the analytic solution for a freezing problem with phase dependent thermal properties showed no significant deterioration of accuracy. Similar performance can be expected with layered systems or problems with rapidly changing boundary conditions.

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TECHNIQUE NUMERIQUE PERFORMANTE POUR DES PROBLEMES THERMIQUES MONODIMENSIONNELS AVEC CHANGEMENT DE PHASE

Résumé—On présente une nouvelle procédure numérique pour traiter les problèmes thermiques monodimensionnels avec changement de phase. La technique qui suit continûment la progression de l'interface de changement de phase est remarquable par sa grande précision obtenue sans sacrifier à la performance de calcul.

WIRKSAMES NUMERISCHES VERFAHREN FÜR EINDIMENSIONALE WÄRMEÜBERTRAGUNGSPROBLEME MIT PHASENWECHSEL

Zusammenfassung—Es wird ein neues numerisches Verfahren für eindimensionale Wärmeübertragungsprobleme mit Phasenänderung vorgestellt. Bei diesem Verfahren wird der Ort der Phasengrenzfläche bei jedem Zeitschritt explizit bestimmt. Der Aufsatz enthält außerdem ein Lösungsverfahren für das Gleichungssystem, das Iterationen in jedem Gitterpunkt vermeidet. Daraus resultiert ein Rechenverfahren, das zugleich numerisch wirkungsvoll und ungewöhnlich genau ist.

ЭФФЕКТИВНЫЙ ЧИСЛЕННЫЙ МЕТОД РЕШЕНИЯ ОДНОМЕРНЫХ ТЕПЛОВЫХ ЗАДАЧ ПРИ ФАЗОВЫХ ПРЕВРАЩЕНИЯХ

Аннотация — В работе представлен новый численный метод решения одномерных задач теплообмена при фазовых превращениях, позволяющий непрерывно определять положение перемещающейся границы раздела фаз. Данный метод обладает высокой точностью и высокой эффективностью при расчётах.