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Goodrich, L. E.
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by L.E. Goodrich

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

L. E. GOODRICH
National Research Council, Canada, Division of Building Research, Geotechnical Section, Ottawa, Ontario, Canada K1A 0R6

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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;
- $L_m$, latent heat per unit volume;
- $S, S'$, Gaussian elimination coefficients, equations (7b), (9b);
- $T$, temperature;
- $t$, time;
- $x$, depth.

Greek symbols
- $\Delta t$, time step;
- $\Delta x$, space interval;
- $\Delta T$, temperature range;
- $\theta$, 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.

EXISTING METHODS

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

$$k_f \frac{\partial T}{\partial x} \bigg|_x - k_u \frac{\partial T}{\partial x} \bigg|_x = (\pm) L \frac{dz}{dt} \quad (1)$$

and

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

at the moving interface. The heat conduction equation

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

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

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

with

$$C_A = C_f \quad \text{for} \quad T > T_f \quad (4a)$$

and

$$C_A = C_f + L_m \frac{\partial \theta}{\partial T} \quad \text{for} \quad T < T_f \quad (4b)$$

where

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

In practice, the entire latent heat is usually associated with a small finite temperature range $\Delta T$ and equation
elemental latent heat source term for inclusion in a
for the phase change interface equation and this
dimension only. It is flexible, but a considerable
amount of computation is required at each time step. The
lent of equation (1) can be used to estimate an
two-dimensional finite-element formulation. The la-
ent heat is considered to be distributed over the
restricts the method to homogeneous media, at the
same time necessitating intricate programming in
and Ehrlich [12] used higher order space differences
iteration, has been proposed by Heitz and Westwater
mulation uses explicit time differencing. A time de-
position of the phase change plane within an element
can be critical when dealing with layered problems
result in a situation in which the $T_f$-isotherm moves
change interface by means of a formulation that
continuously follows the position of the moving phase
change interface. 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 im-
portant. 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
methods that use variable time steps whose length
must be found by nodal iteration, though the for-
mulation uses explicit time differencing. A time de-
pendent 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 equiva-
 lent of equation (1) can be used to estimate an
elemental latent heat source term for inclusion in a
two-dimensional finite-element formulation. The la-
tent heat is considered to be distributed over the

\begin{align}
C_A &= C_J + L_p/\Delta T \quad \text{for} \quad T_f - \Delta T < T < T_f \\
C_A &= C_J \quad \text{for} \quad T < T_f - \Delta T.
\end{align}

The centred time difference equation for layered
systems can be written

\begin{align}
HC_i \cdot (T_i^{m+1} - T_i^m) &= CN_{i-1} \cdot (T_{i-1}^{m+1} - T_{i-1}^m + T_{i-1}^{m+1} + T_{i+1}^m - T_i^m) \\
&+ CN_i \cdot (T_{i+1}^{m+1} - T_{i+1}^m + T_i^{m+1} + T_{i+1}^m - T_i^m) \\
&- 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^{m+1} = RHS_i
\end{align}

where

\begin{align}
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^{m+1}.
\end{align}

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 eli-
mination) yields

\begin{align}
E_0 &= T_0^{m+1} \quad \text{(prescribed)} \\
S_0 &= 0 \\
E_i &= (RHS_i + CN_{i-1} \cdot E_{i-1})/D \quad \text{(7a)} \\
S_i &= CN_i/D \quad \text{(7b)}
\end{align}
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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 \( C_b, k_b \), respectively. Using central differences and assuming \( T_f = 0 \) for convenience, heat balance for node \( i = p \) yields

\[
\frac{1}{2}(C_{p-1} \cdot \Delta x_{p-1} + C_a \cdot H) \cdot \frac{(T_{p+1}^m - T_{p}^m) / \Delta t}{k_a} = \frac{1}{2} k_b \cdot \frac{(T_{p+1}^m + T_{p}^m)}{H} \tag{11}
\]

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

\[
\frac{1}{2}(C_{p+1} \cdot \Delta x_{p+1} + C_b \cdot H) \cdot \frac{(T_{p+1}^m - T_{p+2}^m) / \Delta t}{k_b} = \frac{1}{2} k_a \cdot \frac{(T_{p+1}^m + T_{p+2}^m)}{H} \tag{12}
\]

where

\[ H = \Delta x_{p} - G. \]

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

\[
\pm L_d (G^{m+1} - G^m) / \Delta t + \frac{1}{2} \left( \frac{1}{2} C_a (T_{p+1}^m + T_{p}^m) - \frac{1}{2} C_b (T_{p+1}^m + T_{p+2}^m) \right) = k_a \cdot \left( \frac{T_{p+1}^m + T_{p}^m}{G} \right) + k_b \cdot \left( \frac{T_{p+1}^m + T_{p+2}^m}{H} \right). \tag{13}
\]

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

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

\[
E_p = \frac{CN_{p-1}(T_{m-1}^p + E_{p-1}) + \left( C_{p-1} \frac{\Delta x_{p-1}}{\Delta t} + C_s \frac{G}{\Delta t} - CN_{p-1} - k_b \right) T_p^m}{C_{p-1} \frac{\Delta x_{p-1}}{\Delta t} + C_s \frac{G}{\Delta t} + k_b + CN_{p-1}(1 - S_{p-1})}
\]

and from equation (8)

\[
T_{m+1}^p = S_p \cdot T_f + E_p
\]

or, since

\[
T_f = 0 \\
T_{m+1}^p = E_p
\]

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

\[
T_{m+1}^{p+1} = E_{p+1}
\]

where, following equation (12)

\[
E_{p+1} = \frac{CN_{p+1}(T_{m+2}^p + E_{p+2}) + \left( C_{p+1} \frac{\Delta x_{p+1}}{\Delta t} + C_s \frac{\tilde{H}}{\Delta t} - CN_{p+1} - k_b \frac{\tilde{H}}{\Delta t} \right) T_{p+1}^{m+1}}{C_{p+1} \frac{\Delta x_{p+1}}{\Delta t} + C_s \frac{\tilde{H}}{\Delta t} + k_b + CN_{p+1}(1 - S_{p+2})}
\]

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 \( T_{m+1}^p \) and \( T_{m+1}^{p+1} \) 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

\[
\Delta t_1 = \text{time interval required to move the } T_f\text{-isotherm to the element boundary. Assuming velocity constant over a time step, then whenever equation (13) yields}
\]

\[
G^{m+1} = G' > \Delta x_p
\]

\[
\Delta t_1 \text{ can be approximated by}
\]

\[
\Delta t_1 = \frac{\Delta x_p - G^m}{G - G^{m+1}} \Delta t
\]

Nodal temperatures are updated using the partial time step \( \Delta t_1 \), after which displacement of the phase change

\[
L'' + \frac{CN_{p-1}}{G} \Delta x_{p-1} = \frac{CN_{p-1}}{G} \Delta x_{p-1} + \frac{k_b}{G} + CN_{p-1}(1 - S_{p-1})
\]

\[
\text{VERIFICATION OF THE METHOD}
\]

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:

\[
T(x, 0) = T_{\text{initial}} = +2^\circ C \\
T(0, t) = T_{\text{surface}} = -10^\circ C \quad t > 0 \\
T(\infty, t) = T_{\text{initial}} \quad t \geq 0 \\
k_f = k_t = 2 \text{ W/m} \cdot \text{K} \\
L_s = 100 \text{ MJ/m}^3.
\]

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
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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

\[ k_f = 2.25 \text{ W/m} \cdot \text{K} \]
\[ C_f = 1.5 \text{ MJ/m}^3 \text{K} \]
\[ k_i = 1.75 \text{ W/m} \cdot \text{K} \]
\[ C_i = 2.5 \text{ MJ/m}^3 \text{K} \]

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
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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REFERENCES


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

Résulté—On présente une nouvelle procédure numérique pour traiter les problèmes thermiques monodimensionnels avec changement de phase. La technique qui suit continuellement 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**


**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.