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EFFICIENT NUMERICAL SOLUTION FOR ENTHALPY FORMULATION OF CONDUCTION HEAT TRANSFER WITH PHASE CHANGE

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INTRODUCTION

FORMULATING and solving problems related to heat transfer in systems undergoing phase change continue to occupy the attention of many investigators because of their practical importance in such areas as freezing or thawing of wet soils, solidification or melting of metals, food freezing, and ablation. Judging from the number and nature of the papers that have appeared since 1970, it would appear that analyses of this class of problems are still somewhat ambivalent.

A comprehensive summary of various analytical and numerical techniques that have been used in solving heat conduction with phase change is given by Lunardini [1]. Oddly, he overlooks two significant references: Lukianov and Golovko [2] who pioneered the apparent heat capacity concept and formulation and Hashemi and Sliepcevich [3] who introduced the technique of distributing the latent heat over a finite temperature interval in order to circumvent problems in numerical computation arising from the apparent heat capacity approaching infinity during an instantaneous phase change.

Briefly, two approaches have been used to formulate this class of problems. The first (and still the most familiar) formulation is based on a moving interface or Stefan concept. Unfortunately, the moving interface formulation is not well suited to finite difference or finite element techniques without resorting to complicated techniques such as deforming grids. Another deficiency in the moving interface formulation is the inherent limitation that the entire phase change occurs at a single temperature, whereas in reality for many systems—particularly the freezing of fine grained moist soils—the phase change occurs gradually over a temperature range of several degrees.

The desirability of having a formulation which is applicable for either instantaneous or gradual phase changes prompts a *second* type of formulation, the apparent heat capacity method [2, 3] or its integral, the enthalpy method [4, 5] which includes the latent heat effect in the energy equation. Recent publications on these two formulations employ variations of standard numerical techniques for solving partial differential equations. The principal shortcoming in these approaches is in the application to semi-infinite media which is approximated by assigning an arbitrary magnitude for the extent of this region. Another difficulty encountered in these techniques is the jump discontinuities in the thermophysical properties accompanying an instantaneous phase change. Accordingly, variable grid spacings are required to control the stability of the numerical solution. Thus, Goodrich's criticism [6] that the apparent heat capacity formulation is unacceptable because of oscillations in the numerical results is improper in that the fault really lies with the numerical technique that he used; in fact it can be shown that for his problem the apparent heat capacity formulation leads to stable, accurate results if the numerical techniques as outlined in the following are used.

Briefly, then, the substance of this note is to present a numerical technique for circumventing these aforementioned difficulties. By way of demonstration an enthalpy formulation of the problem of heat conduction with phase change will be solved, specifically the one-dimensional (1-D), semi-infinite Stefan problem.

First, the effect of numerical instabilities can be minimized by expressing the energy equation in dimensionless or normalized variables—regardless of which numerical technique is used to accomplish the calculation.

Second, the accuracy of the numerical computations can be improved by means of a group transformation which reduces the number of variables. In general, this type of transformation is suited to initial value problems; it has limited application for initial-boundary value problems. Specifically, the similarity (Boltzmann) transformation is the only one that works for initial-boundary value problems in the semi-infinite or infinite domains. Although the Boltzmann transformation has been used extensively to obtain *analytical* solutions for special, simple cases of heat conduction with phase change, its value in facilitating numerical solutions of problems for which analytical solutions are not available appears to have been overlooked prior to the study by Anderson and Ford [7]. As pointed out by Crank [8] the Boltzmann transformation does not work for a finite size domain.

In addition to the Boltzmann transformation, an additional transformation or more precisely, coordinate scaling, is used to convert the range of the group variable from 0 to ∞ to the range 0 to 1.

FORMULATION

In the enthalpy method the energy equation for transient heat conduction in Cartesian coordinates is given by

$$\frac{\partial H}{\partial t} = \sum_{i=1}^{N \leq 3} \frac{\partial}{\partial x_i}\left(k\frac{\partial T}{\partial x_i}\right), \tag{1}$$

where t is time, x_i is the Cartesian distance, N is the number of space dimensions, k is thermal conductivity, T is temperature, and H is enthalpy. The variation of enthalpy with respect to temperature is the volumetric heat capacity given by

$$\rho c = \partial H/\partial T. \tag{2}$$

The volumetric heat capacity and the thermal conductivity for a composite system containing a constituent which is partially phase-changed can be predicted using, respectively

$$\rho c = (\rho c)_{\mathrm{tf}} + [(\rho c)_{\mathrm{tu}} - (\rho c)_{\mathrm{tf}}](w_{\mathrm{au}}/w_{\mathrm{ao}}) + \rho_{\mathrm{r}} L_{\mathrm{a}}\, \partial w_{\mathrm{au}}/\partial T, \tag{3}$$

and

$$k = k_{tf} + (k_{tu} - k_{tf})(w_{au}/w_{ao}), \quad (4)$$

in which ρ_r is the density of a reference component in the composite; preferably an inactive component which does not undergo a phase change, w_{au} is the mass of active component which has not yet undergone a phase change per unit mass of reference component, w_{ao} is the total mass of active component originally present per unit mass of reference component, $(\rho c)_{tu}$ and k_{tu} are the volumetric sensible heat capacity and the thermal conductivity, respectively, of the composite (over-all system) which has not undergone any phase change, $(\rho c)_{tf}$ and k_{tf} are the volumetric sensible heat capacity and the thermal conductivity, respectively, of the composite in which the active component has undergone a complete phase change, and L_a is the latent heat of phase change for the active component.

The normalized temperature and enthalpy are defined, respectively, by

$$u = \int_{T_1}^{T} k \, dT \Big/ \int_{T_1}^{T_2} k \, dT, \quad (5)$$

and

$$e = (H - H_1)/(H_2 - H_1), \quad (6)$$

so that equations (1) and (2) become

$$(H_2 - H_1)\frac{\partial e}{\partial t} = \sum_{i=1}^{N \leqslant 3} \frac{\partial}{\partial x_i}\left(\int_{T_1}^{T_2} k \, dT \cdot \frac{\partial u}{\partial x_i}\right), \quad (7)$$

$$\gamma \cdot \rho c = \partial e/\partial u, \quad (8)$$

in which

$$\gamma = \int_{T_1}^{T_2} k \, dT/(H_2 - H_1), \quad (9)$$

where T_1 and T_2 are the range of temperature variation for the system and H_1 and H_2 are the corresponding enthalpy values, respectively.

The dimensionless distance in a given Cartesian direction can be defined by either of the following forms depending on the nature of the problem.

Case I: A finite domain—then the dimensionless distance is

$$y_i = x_i/a_i, \quad (10)$$

where a_i is a characteristic distance in the x_i dimension.

Case II: A semi-infinite domain—then the semi-infinite domain is converted to a unit size finite domain by

$$y_i = 1 - e^{-x_i/a_i}, \quad (11)$$

in which a_i is a geometric scaling factor. This transformation is desirable to avoid uncertainties in representing infinity. For this purpose, Hashemi and Sliepcevich [3] used the transformation $x_i/(1+x_i)$. However, it is more appropriate to use the transformation given by equation (11) since an exponential function is more suited to scale variables extending to infinity.

Case III: A semi-infinite media whose temperature is initially uniform (constant)—then the number of independent variables can be reduced by one using the Boltzmann transformation [8]

$$y_i = x_i/t^{1/2}. \quad (12)$$

Since the Boltzmann transformation still expresses the new variable y_i between zero and infinity, an additional transformation similar to equation (11) is needed to convert the semi-infinite domain to a finite, unit domain. Thus

$$z_i = 1 - e^{-y_i/a_i}, \quad (13)$$

where a_i is some arbitrary scaling factor which should be selected such that better resolution is achieved in the region where the temperature varies more. Applying equations (12) and (13) to equation (7) for a media extending to infinity in all Cartesian coordinates, for example, gives, respectively

$$y_i\frac{\partial e}{\partial y_i} + \frac{2}{(H_2 - H_1)} \sum_{i=1}^{N \leqslant 3} \frac{\partial}{\partial y_i}\left(\int_{T_1}^{T_2} k \, dT \cdot \frac{\partial u}{\partial y_i}\right) = 0, \quad (14)$$

in which the term $y_i \, \partial e/\partial y_i$ can be written in terms of $i = 1, 2,$ or 3, and

$$-(1 - z_i)\ln(1 - z_i)\frac{\partial e}{\partial z_i} + \frac{2}{(H_2 - H_1)} \sum_{i=1}^{N \leqslant 3} (1/a_i^2)(1 - z_i) \times \frac{\partial}{\partial z_i}\left[\int_{T_1}^{T_2} k \, dT \cdot (1 - z_i)\frac{\partial u}{\partial z_i}\right] = 0. \quad (15)$$

APPLICATION

As an example the two-phase Stefan problem for a 1-D system undergoing an instantaneous phase transition will be solved for the case with constant physical properties as used by Goodrich [6]. The results are then compared with the analytical solution given by Carslaw and Jaeger.

The heat transfer is represented by

$$\partial H/\partial t = k \, \partial^2 T/\partial x^2, \quad (16)$$

$$T = T_1, \quad t = 0, \quad 0 \leqslant x < \infty, \quad (17)$$

$$T = T_2, \quad x = 0, \quad t > 0, \quad (18)$$

$$T = T_1, \quad x \to \infty, \quad t > 0. \quad (19)$$

For the 1-D problem considered here, equation (15) is separated into two first-order ordinary differential equations. Thus, equations (16)–(19) reduce to the following:

$$\frac{du}{dz} = \frac{v + \ln(1 - z)e}{2\gamma(1 - z)}, \quad (20)$$

$$u = 1, \quad z = 0, \quad (21)$$

$$u = 0, \quad z = 1, \quad (22)$$

and

$$dv/dz = e/(1 - z). \quad (23)$$

For a solution, the initial value of v is guessed until the final boundary value is obtained. The numerical solution is obtained by integrating the equations simultaneously using a variable step Runge–Kutta–Fehlberg four (five) method requiring that the truncation errors are less than 10^{-12}. An IBM 3081 machine at the University of Oklahoma was used.

The temperature values and the frost depths in terms of the Boltzmann variable obtained via the enthalpy method reproduce those obtained from the exact analytical solution with an average relative error of the order of 10^{-8}.

CONCLUSIONS

Goodrich [6] solves this problem using the apparent heat capacity formulation assuming a freezing range of 0.5°C and employing a Crank–Nicolson method. He compares the frost depth progressing with time with that obtained from Neumann's exact analytical solution. The oscillatory and distorted numerical results reported by Goodrich are due to the use of large step sizes in the Crank–Nicolson method. In addition in his solution the arbitrary value assigned to represent infinite distance probably accounts for some of the accuracy loss in the numerical solution.

The formulation presented in this paper has certain advantages:

(1) The use of dimensionless variables and similarity and scaling transformations not only speeds up the computational process but also improves the accuracy of the results.

(2) Because of the reduction in the number of independent variables the accuracy of the solution can be controlled more efficiently.

(3) The need for representing infinity by approximate

numbers (as required in standard numerical methods) is eliminated by converting the semi-infinite domain to a finite domain.

(4) Even though the dimensionless equation (7) is general, the subsequent transformed equations (14) and (15) are restricted to a semi-infinite domain whose initial temperature is uniform.

(5) In the existence of a convective boundary condition the time variable in the boundary condition equation cannot be eliminated by the Boltzmann transformation. Accordingly, the transformed energy equation needs to be solved repetitively at prescribed time values of the convective boundary condition.

(6) Because the present method combines the space and time variables into one Boltzmann variable, the frost depth is defined by a unique value of the Boltzmann variable at which value the temperature profile has a slope discontinuity.

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