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TECHNICAL NOTES

Effective modeling/analysis of isothermal phase change problems with emphasis on representative enthalpy architectures and finite elements

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INTRODUCTION

THE SUBJECT matter related to phase change and typical of solidification or melting is of importance in many engineering applications. Over the years, a number of analytical and numerical approaches have been attempted for the simulation of phase change problems and a great deal of interest and research endeavors are in progress both in industry and the research community at large.

The purpose of the present paper is to describe effective yet simplified representative enthalpy-based formulations following the initial developments due to the authors [1]. In particular, emphasis on the applicability to a class of isothermal phase change problems is demonstrated via analogous representations with only minor modifications. Although the original developments which we strongly advocate are robust and geared towards the general (isothermal and mushy) phase change problems [1], the present representations provide certain simplifications with some added advantages and restrict attention to a class of isothermal phase change problems. Attention is confined to fixed grid methods for the purposes of illustration.

NUMERICAL MODELS

For the numerical simulation of phase change problems, both finite difference methods and the finite element methods have been extensively used. Because of the inherent flexibility, effectiveness for modeling complex shapes, and the several other advantages, the paper concerns the finite element method. Employing finite elements for modeling/analysis of phase change problems, the class of methods, namely, apparent heat capacity methods, fictitious heat flow or source-based methods, and enthalpy-based methods seem to be the more prominent methods customarily advocated.

The apparent heat capacity methods with temperature fields as the dependent variables have been traditionally used in conjunction with finite elements [2, 3] since the basic form of the equation for phase change is analogous to that of the classical heat conduction equation. However, to handle the Dirac-δ-type behavior for the heat capacity in phase change situations, an enthalpy function is introduced. And various approximations appear in literature for evaluating the effective heat capacity, ρC, of which the more commonly advocated methods are summarized in ref. [1] and references thereof. In conjunction with all of these approximations, a finite interval width $\Delta\theta$ is assumed even for handling isothermal phase change problems. As a consequence of these approximation techniques, a correct heat balance is preserved by avoiding the possibility of missing the peak values, and much of the past work involves interpolation of enthalpy,

$$H = \int \rho c(\theta)\, \mathrm{d}\theta,$$

$H = N_i H_i$, rather than the direct evaluation of the heat capacity.

In the fictitious heat flow or source based methods, the effects due to latent heat are introduced directly as a nonlinear source related term. Most of these methods involve some sort of monitoring of the heat flow to represent the release of latent heat. Numerous strategies have been attempted by various researchers (see Rolph and Bathe [4], Roose and Storrer [5], and references thereof) to include effective updating procedures for computing the resulting liquid fraction field from known temperature fields and the like. Although applicable to isothermal and mushy phase change problems, it has been observed to yield accurate freezing front locations with fairly coarse (large) sizes for mesh and large time steps with the exception for computing temperature fields which require much refined values.

Although enthalpy based methods have been emphasized for phase change problems [6], and literature regarding their use in conjunction with the finite element method is limited (see refs. [7–9]) in comparison to the apparent heat capacity methods, more recently, increased attention has been directed to demonstrate the effectiveness of enthalpy based representations for general phase change problems [1]. The distinguishing differences in the various formulations relevant to enthalpy-based methods lie in the representation of the resulting governing equation either in terms of the total enthalpy and therein employing the discretization process, or, in employing the discretization process firstly in the form represented by

$$\dot{H} - (k_{ij}\theta_{,j})_{,i} = Q \tag{1}$$

and later introducing the representative relations for the temperature θ in terms of the enthalpy H. In this paper it is this later form of representation in which we introduce modifications to our previous efforts to achieve certain added advantages for applicability to a class of isothermal phase change situations.

γ-FAMILY OF REPRESENTATIONS

For handling general phase change problems, we first represent the governing equations in conservation form as

$$H_{,t} = q_{i,i} + Q \quad (x_i, t) \in \Omega X(o, T) \tag{2}$$

subjected to appropriate boundary and initial conditions.

Following our previous effort [1], introducing the approximations

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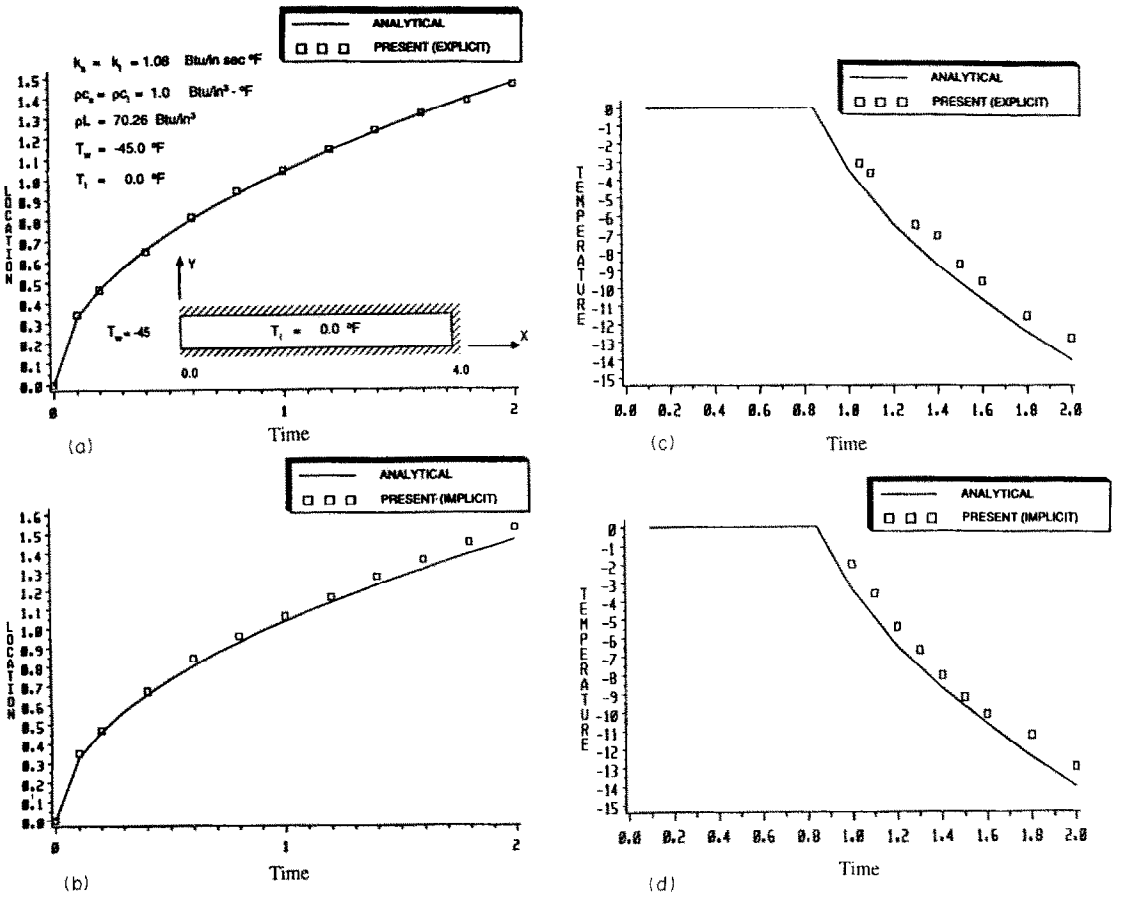

FIG. 1. Comparative freezing front locations and temperature histories for solidification in a semi-infinite slab of liquid. (a) Explicit; (b) implicit; (c) explicit; (d) implicit.

$$H_e(x_i, t) = \mathbf{NH} \tag{3a}$$

$$\mathbf{q}_e = \mathbf{Nq} \tag{3b}$$

the resulting discretized finite element equations for the γ-family of enthalpy representations is obtained following Tamma and Namburu [1] as

$$\mathbf{C}\Delta\mathbf{H}^{n+1} = \mathbf{Q}_1^{n+\gamma} + \mathbf{Q}_2^{n+\gamma} + \mathbf{Q}_3^{n+\gamma} \tag{4}$$

where

$$\Delta\mathbf{H}^{n+1} = \mathbf{H}^{n+1} - \mathbf{H}^n \tag{5}$$

$$\mathbf{C} = \sum_e \Delta t \int_{\Omega_e} N_i N_j \, \mathrm{d}\Omega_e \tag{6a}$$

$$\mathbf{Q}_1^{n+\gamma} = \sum_e \Delta t \int_{\Omega_e} \nabla N_i N_j \, \mathrm{d}\Omega_e \mathbf{q}^{n+\gamma} \tag{6b}$$

$$\mathbf{Q}_2^{n+\gamma} = \sum_e (-\Delta t) \int_{\Gamma_e} N_i N_j \, \mathrm{d}\Gamma_e \mathbf{q}^{n+\gamma} \cdot \hat{n} \tag{6c}$$

$$\mathbf{Q}_3^{n+\gamma} = \sum_e \Delta t \int_{\Omega_e} Q^{n+\gamma} N_i \, \mathrm{d}\Omega_e \tag{6d}$$

and $0 \leqslant \gamma \leqslant 1.0$, where γ is a stability related parameter.

The above γ-family of architectures are representative of the generalized trapezoidal family of schemes. However, they are shown in a different perspective and provide different physical interpretation and various added advantages to significantly enhance the overall effectiveness for general phase change problems (both isothermal and mushy) in comparison to the traditional representations customarily used employing one-step methods [1]. Some of the significant attractive features include: independence of element integrals from material thermophysical properties; permit computation of element integrals only once during the entire analysis; provide effective introduction of general boundary conditions in a direct and natural manner; etc. Technical details are available elsewhere due to Tamma and Namburu [1] and hence are not discussed here.

Since enthalpy is a natural and integral part of the architecture, once the incremental enthalpies are evaluated, we propose an updating approach for evaluating the temperatures via

$$\frac{\mathrm{d}H^{n+\gamma}}{\mathrm{d}\theta^{n+\gamma}} = \rho c|_{\theta^{n+\gamma}} \tag{7}$$

although other analogous approaches are also permissible.

PRESENT MODIFICATIONS WITH PARTICULAR REFERENCE TO ISOTHERMAL PHASE CHANGE PROBLEMS

We next purposely focus attention on a particular form of simplified modifications with some added benefits although restricted to a class of isothermal phase change problems because of the particular temperature-enthalpy relations employed. In particular, we herein retain all of the significant attractive features of the original γ-family of representations and therein additionally demonstrate some added advantages as described subsequently.

The fundamental modifications we introduce lie in the handling of the heat flux vector $\mathbf{q}^{n+\gamma}$ (which is normally evaluated employing Fourier's law and finite element approximations) appearing in the discretized equations (equations (6)).

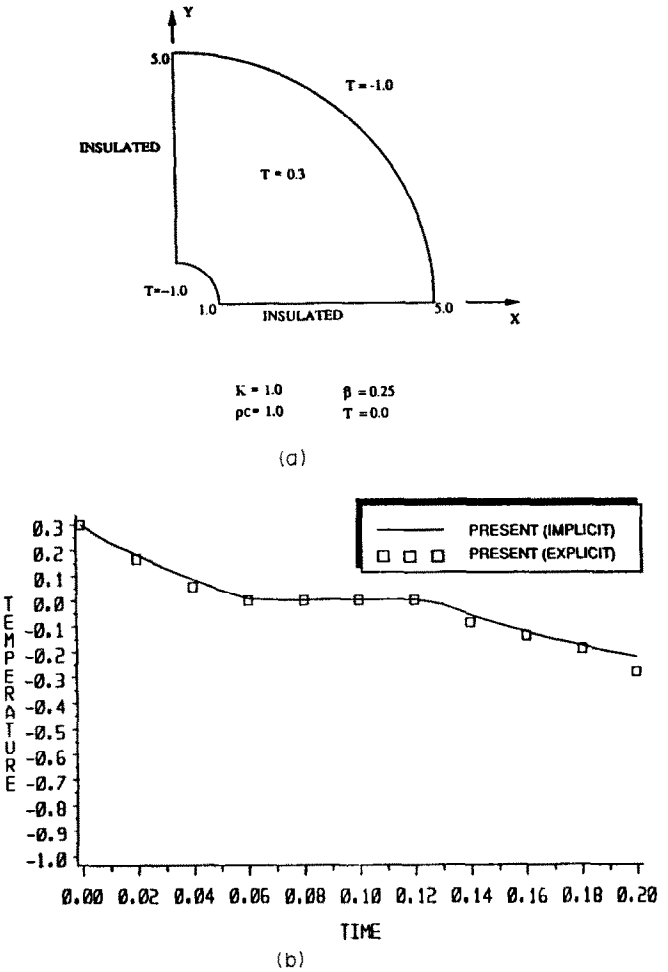

FIG. 2. Solidification of a circular region. (a) Description of model and data; (b) comparative explicit and implicit temperature histories ($x = 0.98$, $y = 1.0$).

For the class of isothermal phase change problems considered, the temperature θ and enthalpy H are related as follows:

$$\theta = \begin{cases} \dfrac{H}{\rho c} & H < \rho c < \theta_m \\ \theta_m & c\theta_m \leqslant H \leqslant \rho c\theta_m \\ \dfrac{(H-L)}{\rho c} & H > \rho c\theta_m + L \end{cases} \tag{8}$$

where θ_m is the melting/freezing temperature.

The heat flux vector employing Fourier's law is given as

$$\mathbf{q} = -k_{ij}\theta_{,j}. \tag{9}$$

Instead of introducing the temperature interpolation approximations in the above, we propose to employ the temperature–enthalpy relations by equation (8), where the finite element approximations for enthalpy are represented as

$$H_e = \mathbf{NH}. \tag{10}$$

For isothermal phase change problems, equations (4) are solved for the enthalpy first. Therein, temperatures are merely obtained as a result of a simple post-processing operation by employing the temperature–enthalpy relations, equations (8), shown previously.

The added advantages via the present modifications for isothermal phase change problems include the following considerations:

permits larger time steps for the present implicit counterpart;

obviates the need to introduce an artificial finite width interval '$\Delta\theta$' for isothermal phase change situations;

eliminates the need for averaging approximations for the effective heat capacity;

enables a good approximation for the location of the phase front.

All of the other distinguishing characteristics of the γ-family of representations outlined previously and described elsewhere by Tamma and Namburu [1] for general solidification problems are retained.

In comparison to ref. [1], a disadvantage by introducing the present modifications is that for the implicit solution procedure, the resulting Jacobian matrix involved with the Newton–Raphson procedure is unsymmetrical.

ILLUSTRATIVE EXAMPLES

Test case 1: *solidification of a semi-infinite slab of liquid*

The geometry and relevant data for the model is depicted

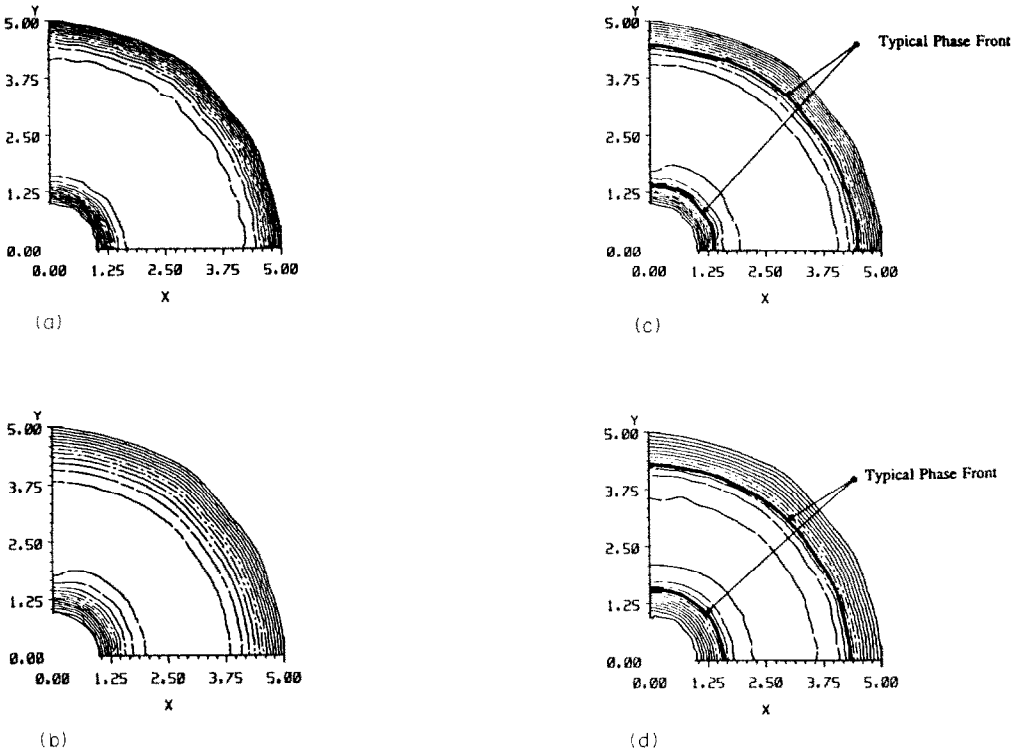

FIG. 3. Solidification of a circular region. (a) Temperature contours, $t = 0.1$ s; (b) temperature contours, $t = 0.2$ s; (c) enthalpy contours, $t = 0.1$ s; (d) enthalpy contours, $t = 0.2$ s.

in Fig. 1(a). As shown, the uniform infinite slab of liquid initially at zero temperature, is subjected to a temperature of -45 F at the left end and is held constant. This test model examines the solidification of a semi-infinite slab of liquid and an analytical solution exists [1, 10].

The problem is modeled employing four-noded bilinear elements (40 elements). The problem is analyzed using the explicit ($\gamma = 0$) and the implicit ($\gamma = 1$) representations. A lumped capacitance matrix is employed for all calculations. The comparative locations of the phase front and temperature histories at a location $x = 1$ are shown in Figs. 1(a)–(d). The present simulations agree very well with the analytical results. The computational ratio for the present explicit to the implicit forms is 1 : 1.53.

Test case 2: *solidification of a circular region*

This test model proposes a two dimensional circular region with a circular hole which is initially at $T_i = 0.3$, while the exposed edges are maintained at $T = -1.0$. Due to symmetry considerations, only a quarter of the region is modeled and a description of the problem is shown in Fig. 2(a). The problem is modeled employing 100 four-noded bilinear elements. The comparative temperature histories are shown for the explicit and the implicit forms in Fig. 2(b) for a typical point located at $x = 0.98$ and $y = 1.0$. Typical temperature contours at time 0.1 and 0.2 s are shown in Figs. 3(a),(b) for the explicit form. Unlike the previous representations, Figs. 3(c),(d) show contours of enthalpies for the implicit form at time 0.1 and 0.2 s respectively. Typical locations of the phase front are shown in the above contour plots (Figs. 3(c),(d)) at time 0.1 and 0.2 s respectively. The computational ratio for the explicit to the implicit forms is 1 : 1.32.

CONCLUDING REMARKS

An effective modeling/analysis approach based on a generalized γ-family of representations with emphasis on representative enthalpy architectures was described with special reference to a class of isothermal phase change applications. In particular, introducing minor modifications, the present form of representations obviate the need to introduce a finite interval width, thereby overcoming any type of approximations for representing strict isothermal phase change situations. Averaging approximations are also not involved and larger time steps are permissible for the time integrations. The present explicit form is also clearly superior to the present implicit form. In comparison to other analogous finite element approaches traditionally followed for similar problems, the present explicit and implicit formulations should compete extremely well (based on our previous comparative research efforts [1] for general phase change problems). The overall results indicate good agreement and the proposed formulations provide an effective methodology for a class of isothermal phase change problems.

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Steady state multiplicity in boiling fluid pipe flow

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1. INTRODUCTION

THE PROBLEM considered is that of a pipe in which flows a fluid that may evaporate. A uniform heat flux is supplied along the pipe and is independent of the flow rate inside the pipe. This may be the case in nuclear reactor cores, in electrically heated tubes or as an approximation in cases where the pipe is heated by radiation by high temperature flames. The fluid enters the pipe as a sub-cooled liquid and exits the pipe as a liquid–vapor mixture. An increase in the mass flow rate causes both an increase in the frictional pressure drop and a decrease in the length of the two-phase zone, and in the exit vapor fraction, causing a smaller change in momentum flux. These conflicting effects result in the possibility of a local maximum in the variation of pressure drop with flow rate, as will be shown later.

2. ANALYTICAL MODEL

In order to understand the physics of the phenomenon, we shall first develop a simplified approximation, for which an analytical solution can be derived. This will then be compared with a numerical simulation of the system described. The assumptions of the model are:

(a) Liquid and vapor properties are constants (ΔH_{LV}, ΔV_{LV}, V_L, C_{PL}).
(b) The pressure drop is small and therefore the saturation temperature, T_s, is constant.
(c) The liquid viscosity is constant and the two-phase mixture viscosity is equal to the liquid viscosity.
(d) The flow is turbulent and the friction factor is described by the Blasius approximation: $f_f = 0.079\,Re^{-0.25}$.
(e) The two-phase flow is described by the homogeneous flow model.
(f) The heat input to the pipe, q_{in}, is uniform.
(g) The flow is one dimensional (no radial changes).
(h) Axial heat conduction is neglected.
(i) In the two-phase zone, the fluid is in equilibrium at all points.
(j) Steady state conditions are assumed throughout.

We note that assumptions (a)–(c) above do not apply to the numerical simulations brought in Section 3. The two model equations are:

Energy balance:

$$\dot{m}\frac{dH}{dl} = q_{in} \tag{1}$$

In the liquid zone:

$$\frac{dH}{dl} = C_{PL}\frac{dT}{dl} \tag{1a}$$

In the two-phase zone:

$$\frac{dH}{dl} = \Delta H_{LV}\frac{d\langle x\rangle}{dl} \tag{1b}$$

Momentum balance:

$$\frac{dP}{dl} = \frac{dP_f}{dl} + \frac{dP_a}{dl}. \tag{2}$$

Here, the terms on the right hand side are the frictional pressure gradient:

$$\frac{dP_f}{dl} = -2f_f\frac{\rho u^2}{D}, \tag{3}$$

and the pressure gradient due to acceleration:

$$\frac{dP_a}{dl} = -\frac{d}{dl}(\langle \rho u^2\rangle). \tag{4}$$

These can be expressed in terms of $\dot{m}$: $\rho u = \dot{G} = \dot{m}/A$; $\rho u^2 = \dot{G}^2/\rho = \dot{m}^2/A^2\cdot\langle V\rangle$; $Re = 4\dot{m}/\pi D\mu$. In the two-phase region:

$$\langle V\rangle = V_L + \langle x\rangle\Delta V_{LV},$$

and

$$\frac{d\langle V\rangle}{dl} = \Delta V_{LV}\frac{d\langle x\rangle}{dl}.$$

From (1) and (1b):

$$\frac{d\langle x\rangle}{dl} = \frac{q_{in}}{\dot{m}\Delta H_{LV}}.$$

Substituting into (4) gives:

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