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ON ADAPTIVE TIME STEPPING APPROACHES FOR THERMAL SOLIDIFICATION PROCESSES

TIANHONG OUYANG AND KUMAR K. TAMMA

Department of Mechanical Engineering, 111 Church St. S.E., University of Minnesota, Minneapolis, MN 55455

ABSTRACT

Thermal solidification processes are an important concern in today's manufacturing technology. Because of the complex geometric nature of real-world problems, analytical techniques with closed-form solutions are scarce and/or not feasible. As a consequence, various numerical techniques have been employed for the numerical simulations. Of interest in the present paper are thermal solidification problems involving single or multiple arbitary phases. In order to effectively handle such problems, the finite element method is employed in conjunction with adaptive time stepping approaches to accurately and effectively track the various phase fronts and describe the physics of phase front interactions and thermal behaviour. In conjunction with the enthalpy method which is employed to handle the latent heat release, a fixed-grid finite element technique and an automatic time stepping approach which uses the norm of the temperature distribution differences between adjacent time step levels to control the error are employed with the scale of the norm being automatically selected. Several numerical examples, including single and multiple phase change problems, are described.

KEY WORDS Adaptive schemes Solidification Finite element

INTRODUCTION

Solidification processes are of importance in today's manufacturing technology. During the past two decades, it has seen extensive interest and activity in the modelling and analysis of numerous applications in solidification processes[1–17]. Various techniques have been employed including analytical and numerical methods. Because of the complexity of real world problems, numerical techniques can be seen to be well suited for the computational simulation of solidification problems. Traditionally, the finite difference method (FDM) has been used. But, during the last twenty years, a widespread interest has been shown in the finite element method (FEM) for such problems. Due to the ability of FEM to handle complex geometries and boundaries, the ease in implementing arbitrary boundary conditions, and the capability of being implemented in a flexible general purpose manner, it is the chosen method in this paper. Although many investigations of solidification involve a single phase change situation, the simultaneous co-existence of multiple phases increases the complexity and also has applications to several practical engineering problems.

For the transient analysis in the simulation of solidification processes, it is well known that it may be a difficult task to choose proper and optimal time steps for the integration of the associated transient heat transfer problem in practical applications. The task of choosing the proper time step has often been considered as being a matter of experience and, in most of cases, simply a uniform time step, i.e. time step $\Delta t = \text{constant}$, has been traditionally employed in the computational simulations. Approaches to involve mixed time integration have also been

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attempted[18] but for single phase change situations. Much of the past work in conjunction with finite elements has mostly focused attention on single phase change situations. More recent efforts by Ouyang and Tamma[19,20] show new finite element developments to handle multiple-phase front situations which are important in several practical problems. However, attention was confined to only a single uniform time stepping strategy. The development of efficient strategies for automatic time stepping which arise in transient finite element analysis of phase change problems is an important area of research and has significant potential for practical applications since it is well known that efficient strategies make good use of computational resources and allow more complex solution algorithms to be effectively studied.

The present work is concerned with and permits solidification processes, including an arbitrary number of multiple phases to co-exist simultaneously, in phase change problems. To accurately predict the solution behaviour and to effectively make good use of the computational resources, adaptive step-size selection strategies are considered for solidification problems involving phase change. The robustness of such strategies for nonlinear transient problems not only requires a theoretically sound approach but also requires an efficient implementation and evaluation procedure to determine the viability for practical applications. Adaptive algorithms are now entering into applications and adaptivity in both time selection and space sizing may be expected to become a standard feature of the FEM in the future. Qualitative error control is of obvious interest in applications, and efficient techniques for adaptive algorithms open doors for fascinating possibilities of computing accurate solutions to complex problems at optimal computational cost.

For parabolic problems, Eriksson and Johnson[21] and Johnson *et al.*[22] introduced an automatic time stepping method by controlling the differences of dependent variable variation between adjacent time step levels. The approach was based on a posteriori error estimates and gives control of the global error. For a single change situation, Tadayon *et al.*[18] describe an implicit-explicit approach for transient heat conduction analysis.

In the present paper, for applications to solidification processes involving single phase or the simultaneous co-existence of arbitrary number of phases, in conjunction with the enthalpy method which is employed to handle the latent heat release and a fixed-grid finite element technique for providing simplicity in the computations, an automatic time stepping approach is used. This employs the norm of the temperature distribution differences between adjacent time step levels to control errors for effectively and accurately simulating the transient behaviour and location of the phase fronts. Several numerical examples, including one and two-dimensional problems involving single and multiple phase change problems, are presented.

THE GOVERNING MODEL EQUATIONS

We consider the nonlinear transient heat conduction problem involving phase change where we seek to find $T = T(x_1, \ldots, x_d, t)$, such that

$$\rho c \frac{\partial T}{\partial t} - \nabla.(k \nabla T) = Q \qquad \text{in } \Omega,\ t>0 \quad \text{(1.a)}$$

$$T = T_p \qquad \text{on } \partial\Omega_x,\ t>0 \text{(1.b)}$$

$$-q_i n_i = \beta \qquad \text{on } \partial\Omega_\beta,\ t>0 \text{(1.c)}$$

$$T(\bullet, 0) = T_0 \qquad \text{in } \Omega \quad \text{(1.d)}$$

where the heat flux is defined as,

$$q_i = -k_{ij} T_{,j} \qquad \text{(1.e)}$$

Equation (1) represents a typical nonlinear transient heat conduction problem involving phase change, where T represents the temperature and d is the number of spatial dimensions. Ω is the

bounded domain in R^d with arbitrary boundary $\partial\Omega=\partial\Omega_x\cup\partial\Omega_\beta$ and $\partial\Omega_x\cap\partial\Omega_\beta=0$. Q, β, T_p, and T_0 are given functions. k is the thermal conductivity, ρ and c are the density and specific heat, respectively. In general, they may be functions of T, i.e.,

$$\rho=\rho(T), \qquad c=c(T) \qquad \text{and} \qquad k=k(T) \tag{2.a}$$

We assume that the heat capacity ρc and thermal conductivity k are bounded, i.e., there exist constants C_1 and C_2 such that,

$$\rho c(x)\leqslant C_1, \qquad k(x)\leqslant C_2 \qquad \forall\, x\in\Omega \tag{2.b}$$

We describe later the use of enthalpy formulations for treatment of the effective heat capacity, ρc in phase change problems. In particular by defining an enthalpy function,

$$H=\int_{T_0}^{T}\rho c(T)\,\mathrm{d}T \tag{2.c}$$

where T_0 is a reference temperature.

NUMERICAL FORMULATIONS

Weak formulation

Denoting,

$$\nabla T=\left(\frac{\partial T}{\partial x_1},\ldots,\frac{\partial T}{\partial x_d}\right) \tag{3}$$

The set of trial and weighting functions are given as,

$$\Psi=\{T\,|\,T\in H^1(\Omega),\ T=T_p \text{ on } \partial\Omega_x\} \tag{4.a}$$

$$\mathcal{V}=\{w\,|\,w\in H^1(\Omega),\ w=0 \text{ on } \partial\Omega_x\} \tag{4.b}$$

where $H^1(\Omega)$ is the Hilbert space. For positive constants C_1, C_2, the problem can now be given the following equivalent weak formulation,

For given T_0, find $T\in\Psi\times I$ such that $\forall\, w\in\mathcal{V}$

$$(\rho c\dot{T},\mathrm{w})+(k\nabla T,\nabla w)=(Q,w)+(\beta,w)_{\partial\Omega_\beta} \tag{5}$$

$\dot{T}$ denotes the derivative of T with respect to time, $(\bullet,\bullet)$ denotes the usual inner product, and $I=[0,t]$ denotes the time domain, ρc the heat capacity.

Galerkin formulation

Denoting $\mathcal{V}^h$ and Ψ^h be a finite-dimensional subspace of $\mathcal{V}$ and Ψ, i.e.

$$\mathcal{V}^h\subset\mathcal{V} \tag{6.a}$$

$$\Psi^h\subset\Psi \tag{6.b}$$

where h is the scale of mesh size, the Galerkin formulation may be stated as,

Find $T^h\in\Psi^h(\Omega)\times I$ such that $\forall\, w^h\in\mathcal{V}^h$

$$(\rho c\dot{T}^h,w^h)+(k\nabla T^h,\nabla w^h)=(Q,w^h)+(\beta,w^h)_{\partial\Omega_\beta} \tag{6.c}$$

Finite element formulation

Let us divide the region into E elements with N nodes and represent T^h in terms of basis function,

$$T^h(x, t)=\sum_{j=1}^{N} \Phi_j(x)T_j(t) \tag{7}$$

where Φ is the basis function and x represents $(x_1, \ldots, x_d)$.

The matrix formulation may be defined as,

Find $T_j \in R^N$ such that

$$M_{ij}\dot{T}_j+K_{ij}T_j=Q_i \qquad t\in(0, t_n) \quad i, j=1, 2, \ldots, N \quad \text{sum on } j \tag{8.a}$$

$$T(0)=T_0 \tag{8.b}$$

where $(0, t_n)$ is the time domain and,

$$M_{ij}=\sum_{e=1}^{E} m_{ij}^e=\sum_{e=1}^{E}\int_{\Omega^e} C_a\Phi_i(x)\Phi_j(x)\,\mathrm{d}\Omega \tag{9.a}$$

$$K_{ij}=\sum_{e=1}^{E} k_{ij}^e=\sum_{e=1}^{E}\int_{\Omega_e} k\,\nabla\Phi_i(x)\,\nabla\Phi_j(x)\,\mathrm{d}\Omega \tag{9.b}$$

$$Q_i=\sum_{e=1}^{E} Q_i^e=\sum_{e=1}^{E}\int_{\Omega_e} \Phi_i(x)Q\,\mathrm{d}\Omega-\int_{\partial\Omega_\beta} \Phi_i(x)\beta\,\mathrm{d}\partial\Omega_\beta \tag{9.c}$$

where the approximation for C_a is defined in (16) and the enthalpy formulation is introduced.

TIME INTEGRATION

The α-family of trapezoid methods has been used for the time integration[23].

$$\boldsymbol{M}^{n+\alpha}[(\boldsymbol{T}^{n+1}-{}^n)/\Delta t]+\boldsymbol{K}^{n+\alpha}[\alpha\boldsymbol{T}^{n+1}+(1-\alpha)\boldsymbol{T}^n]=\boldsymbol{Q}^{n+\alpha} \tag{10}$$

where Δt is the time step and α is the integration parameter defined as $0\leqslant\alpha\leqslant 1$. $\alpha\geqslant 0.5$ is used in the present work for which unconditional stability exists. The thermal properties are evaluated at time $n+\alpha$, i.e.,

$$t_{n+\alpha}=(1-\alpha)t_n+\alpha t_{n+1} \tag{11}$$

where $t_n=n\,\Delta t$ and $t_{n+1}=(n+1)\,\Delta t$. A lumped capacitance matrix $\boldsymbol{M}$ is used in (10). Note that, when $\alpha\neq 0$, a Newton-Raphson type iteration is employed to compute $\boldsymbol{T}^{n+1}$.

ENTHALPY FORMULATION

For solidification processes, for certain materials the phenomenon of phase change occurs over a wide band of temperature ranges. Such problems permit fairly reasonable approximations for physically modelling the situation. However, for several other materials, the phase change phenomenon takes place instantaneously with almost no temperature variation and are characterized by a Dirac-δ-type behaviour. These problems are somewhat more difficult computationally.

The evolution of latent heat can be treated in terms of the thermophysical parameters, i.e. heat capacity ρc, which is temperature dependent. The enthalpy method is an effective approach and a common practice to simulate the Stefan problem employing fixed-grids. The most significant difference between the enthalpy method and other methods is the formulation of the element heat capacitance on the heat-storage matrix $\boldsymbol{M}^e$. For the fixed-grid system, where the solidification front position is generally at an unknown location between nodes, the enthalpy method treats

matrix M^e of the elements. An effective specific heat for an entire element through the use of the enthalpy function H is calculated. The freezing front flux condition is incorporated into a new form of the governing equations that is valid over the whole fixed domain (solid and liquid). The front locations are calculated after solving the problem using postprocessing operations. As a consequence, introducing the enthalpy formulation for effectively handling phase change problems, we define the enthalpy function,

$$H=\int_{T_0}^{T}\rho c(T)\,\mathrm{d}T \tag{12}$$

where the T_0 is a reference temperature. For the Stefan problem, one can write

$$H=\int_{T_0}^{T}\rho c_s(T)\,\mathrm{d}T \qquad (T<T_m) \tag{13.a}$$

$$H=\int_{T_0}^{T_m}\rho c_s(T)\,\mathrm{d}T+\rho\mathscr{L}+\int_{T_m}^{T}\rho c_L(T)\,\mathrm{d}T \qquad (T\geqslant T_m) \tag{13.b}$$

where $\mathscr{L}$ is the latent heat while the subscripts s and L represent solid and liquid phase, respectively. T_m is the melting temperature. In the numerical implementation this direct evaluation requires spreading the phase change across a temperature interval and thus introducing a freezing range. This freezing range must be kept small to avoid too much deviation from the original phase change problem (Stefan problem). For the finite freezing interval $[T_m-\Delta T, T_m+\Delta T]$, the enthalpy may be defined,

$$H=\int_{T_o}^{T}\rho_s c_s(T)\,\mathrm{d}T \qquad (T<T_{m1}) \tag{14.a}$$

$$H=\int_{T_0}^{T_{m1}}\rho_s c_s(T)\,\mathrm{d}T+\int_{T_{m1}}^{T}\left[\rho_m\frac{\mathscr{L}}{2\Delta T}+\rho_m c_m(T)\right]\mathrm{d}T \qquad (T_{m1}<T<T_{m2}) \tag{14.b}$$

$$H=\int_{T_0}^{T_{m1}}\rho_s c_s(T)\,\mathrm{d}T+\rho_m\mathscr{L}+\int_{T_{m1}}^{T_{m2}}\rho_m c_m(T)\,\mathrm{d}T+\int_{T_{m2}}^{T}\rho_L c_L(T)\,\mathrm{d}T \qquad (T>T_{m2}) \tag{14.c}$$

where $T_{m1}=T_m-\Delta T$ and $T_{m2}=T_m+\Delta T$ and ΔT is a half-temperature range over which phase change occurs. The quantities $c_m=\frac{1}{2}(c_S+c_L)$ and $\rho_m=\frac{1}{2}(\rho_S+\rho_L)$ are the specific heat and density in the freezing interval.

With the above definition of the enthalpy function, the effective heat capacity may be defined as

$$\rho c(T)=\frac{dH}{\mathrm{d}T} \tag{15}$$

Because H is a unique function of temperature, the governing mathematical model equation involving phase change may be stated as,

$$C_a\frac{\partial T}{\partial t}-\nabla.(k\nabla T)=Q \tag{16}$$

where $C_a=(\mathrm{d}H/\mathrm{d}T)$.

In the numerical simulation of phase change problems, approximating the term C_a in the element capacitance matrix M^e is a critical step. Various approximation methods have been suggested and they are well documented in References 15 and 16. In the present study, we restrict attention to that due to Del Guidice *et al.*[3] which has been cited to yield satisfactory results

and also based on our past experiences[16,17,19,20],

$$C_a=\frac{\left[\left(\frac{\partial H}{\partial x}\right)\left(\frac{\partial T}{\partial x}\right)+\left(\frac{\partial H}{\partial y}\right)\left(\frac{\partial T}{\partial y}\right)+\left(\frac{\partial H}{\partial z}\right)\left(\frac{\partial T}{\partial z}\right)\right]}{\left[\left(\frac{\partial T}{\partial x}\right)^2+\left(\frac{\partial T}{\partial y}\right)^2+\left(\frac{\partial T}{\partial z}\right)^2\right]} \tag{17}$$

ADAPTIVE TIME STEPPING STRATEGY FOR SOLIDIFICATION PROCESSES

The adaptive strategy described for applications to solidification problems involving phase change follows next and employs an automatic error control and solution approach. The nonlinear transient heat conduction problem involving phase change (16) can be given the following equivalent weak form. For a given T_0,

Find $T\in\Psi\times I$ such that $\forall\, v\in\mathcal{Y}$

$$(C_a\dot{T}(t), v)+(k(T(t))\nabla T(t), \nabla v)=(Q(t), v)+(\beta, v)_{\partial\Omega_\beta} \tag{18.a}$$

$$T(0)=T_0 \tag{18.b}$$

For the discretization in time, let $0=t_0<t_1<\cdots<t_m<\cdots<t_n$, and $I_m(t_{m-1}, t_m]$, $\Delta t_m=t_m-t_{m-1}$, where n is the total number of time steps.

So the problem becomes,

Fing T such that $\forall\, v\in\mathcal{Y}$

$$\int_{I_m}\{(C_a\dot{T}, v)+(k(T)\nabla T, \nabla v)\}\,\mathrm{d}t=\int_{I_m}(Q(t), v)\,\mathrm{d}t+(\beta, v)_{\partial\Omega_\beta}\,\mathrm{d}t \tag{19.a}$$

$$T(0)=T_0 \tag{19.b}$$

Since $\Delta t_m=t_m-t_{m-1}$, the problem can be rewritten as,

$$(C_a(T_m-T_{m-1}), v)+\Delta t_m(k(T)\nabla T(t), \nabla v)=\int_{I_m}(Q(t), v)\,\mathrm{d}t+(\beta, v)_{\partial\Omega_\beta}\,\mathrm{d}t \tag{20}$$

The adaptive strategy follows that proposed by Eriksson and Johnson[21] for nonlinear parabolic problems, where, for a given tolerance $\delta>0$, we can select the time step Δt_m, $m=1, 2, \ldots, n$ such that,

$$C\,\Delta t\max_{t\leqslant t_n}\|\dot{T}\|\approx\delta \tag{21.a}$$

or

$$\|T_m-T_{m-1}\|_\infty\approx\frac{\delta}{C}=\Delta_{Tol} \tag{21.b}$$

where C is a constant. The discrete solution satisfies,

$$\max_{t\leqslant t_n}\|T_{exact}(t)-T(t)\|_\infty\leqslant\delta \tag{22}$$

As a consequence, assuming that T_{m-1} has been computed and q is a suitable constant (>1, and may be problem dependent), the following steps are then used to select Δt:

(1) choose $\Delta t_m=\Delta t_{m-1}$
(2) calculate T_m by Δt_m
(3) if

$\frac{1}{q}\Delta_{Tol} \leqslant \| T_m - T_{m-1} \|_\infty \leqslant \Delta_{Tol}$ (where Δ_{Tol} is a user prescribed quantity)

then accept time step Δt_m and go on next time step, otherwise decrease or increase Δt_m by a factor F (user selected) and repeat the procedure started at (2).

The estimated error employing the above is thus,

$$\max_{t \leqslant t_n} \| T_{exact}(t) - T(t) \|_\infty \leqslant \delta = C\,\Delta_{Tol} \tag{23}$$

That is,

$$\| T_{exact}(t) - T(t) \|_\infty \leqslant \delta \tag{24}$$

The above time stepping strategy for phase change situations is theoretically justified (due to Eriksson and Johnson[21] and Johnson[22]) and can provide a posteriori error estimation. The cost of the time step control is considerably small. Since the implicit form of the methods are unconditionally stable when $\alpha \geqslant 0.5$, the cirterion for selection of adaptive time steps is that based on accuracy issues.

For the adaptive time stepping strategy, Δ_{Tol} can also be automatically selected to control the error employing the following proposed procedure:

(1) Set the initial guess for $\Delta^0_{Tol} \times x\% T_r$, where T_r is the temperature range defined as $T_r = |T_0 - T_p|$ in this work. Then compute the temperature distribution ${}^0T$ according to Δ^0_{Tol} for the time range $t_i = y\% t_n$.

(2) Set $\Delta^1_{Tol} = z\Delta^0_{Tol}$, where z is a constant, and compute the temperature distribution ${}^1T$ for Δ^1_{Tol} for $t_i = y\% t_n$.

(3) If

$$\frac{\| {}^0T - {}^1T \|_\infty}{T_r} \leqslant \varepsilon_{\text{tolerance}} \tag{25}$$

then Δ^0_{Tol} is selected. Otherwise set $\Delta^0_{Tol} = \Delta^1_{Tol}$ and ${}^0T = {}^1T$, and the procedure started from step (2) is repeated until (25) is satisfied. It should be noted that the parameters x, y, z and $\varepsilon_{\text{tolerance}}$ are normally user specified quantities and tolerance levels for accuracy considerations.

For certain types of problems it may be necessary to prescribe bounds for the time steps. For instance, in some cases it may be necessary to limit the time step by an upper value Δt_{max} in order to permit tracing of the temperature history in a certain time interval, while in other cases it may be necessary to ensure that the time steps do not go below a prescribed lower limit Δt_{min} in order to prevent excessive computational costs. The time stepping is adaptively controlled and the computational effort involved in adaptively adjusting the time steps following the present procedure is relatively small in comparison to employing a uniform constant stepping approach. Since the adaptive strategy is based on a posteriori error estimates, it follows that the algorithm is reliable in the above sense, and for $\| T_{exact} - T \|_\infty < \delta$ the error is bounded. The above mentioned approach enables control of the error and permits an efficient and optimal strategy for the numerical simulation of solidification processes involving the co-existence of arbitrary number of phases. This is demonstrated in the following section.

NUMERICAL EXAMPLES

Several numerical one-dimensional and two-dimensional test examples in thermal problems involving single and multiple phase change situations are presented in this section. An automatic time stepping strategy with qualitative error control is employed for the applications and the trapezoidal α-family of methods ($\alpha \geqslant 0.5$) is used. Whenever feasible, the numerical solutions are compared with an analytical solution as in the first and third example for single phase change situations, while the results presented for multiple phase front situations have been validated (not shown here) with those involving a single uniform time stepping strategy.

Table 1 Thermal properties of water

Heat conductivity in solid k_S	2.179 W/m-K
Heat conductivity in liquid k_L	0.588 W/m-K
Specific heat in solid c_S	1966.48 J/kg-K
Specific heat in liquid c_L	4184.00 J/kg-K
Density in solid ρ_S	921.1 kg/m^3
Density in liquid ρ_L	999.6 kg/m^3
Latent heat $\mathscr{L}$	334720 J/kg
Melting temperature T_m	273 K

One-dimensional single phase change problem

In this example, solidification in a one-dimensional semi-infinite region is studied. Initially, the region is considered to be liquid which is at a temperature higher than the melting temperature T_m. The material properties are given in *Table 1*.

The initial and boundary conditions for the example are as follows,

$$T(x, 0)=328.56\ \text{K},\ T(0, t)=217.44\ \text{K},\ T(\infty, t)=328.56\ \text{K}$$

The analytical solution of this problem can be found in the book by Luikov[24], but has been derived by Stefan in 1899,

$$T_{exact}(x, t)=T(0, t)+\frac{T_m-T(0, t)}{\text{erf}(\lambda)}\,\text{erf}\left(\frac{x}{2}\sqrt{\frac{\rho_S c_S}{k_S t}}\right) \qquad 0<x<h(t) \tag{26.a}$$

$$T_{exact}(x, t)=T(x, 0)-\frac{T(x, 0)-T_m}{\text{erfc}\left(\lambda\sqrt{\frac{k_S\rho_L c_L}{k_L\rho_S c_S}}\right)}\,\text{erfc}\left(\frac{x}{2}\sqrt{\frac{\rho_L c_L}{k_L t}}\right) \qquad h(t)<x \tag{26.b}$$

where erf is the error function and the erfc is the complementary error function while the front position is,

$$h(t)=2\lambda\sqrt{\frac{k_S t}{\rho_S c_S}} \tag{26.c}$$

The value of λ is determined by solving the following characteristic equation,

$$\sqrt{k_S\rho_S c_S}\,[T_m-T(0, t)]\,\frac{\exp(-\lambda^2)}{\text{erf}(\lambda)}-\sqrt{k_L\rho_L c_L}\,[T(x, 0)-T_m]\,\frac{\exp\left(-\lambda^2\frac{k_S\rho_L c_L}{k_L\rho_S c_S}\right)}{\text{erfc}\left(\lambda\sqrt{\frac{k_S\rho_L c_L}{k_L\rho_S c_S}}\right)}=\lambda\mathscr{L}\sqrt{\pi}\sqrt{\frac{k_S}{\rho_S c_S}} \tag{26.d}$$

In the finite element analysis, a finite domain $0<x<l$ is used and only the solution at early time is considered to represent the semi-infinite slab. Twenty linear finite elements are used in this simulation and the length of the region is $l=5.08$ (cm). The integration parameter $\alpha=1$ in (10) is used and the heat capacitance is lumped.

Figure 1 gives the comparative front positions for the analytical and present solution. *Figure 2* shows the adaptive time step history. It can be seen that the time step is automatically adjusted. During the early stage of the simulation, the time step is small since the temperature changed dramatically near $x=0$ where the sudden temperature boundary condition is applied. With time lapse, the temperature distribution is not as steep, so the time step is automatically adjusted to larger values. Efficient time stepping methods for computing the representative solution of such

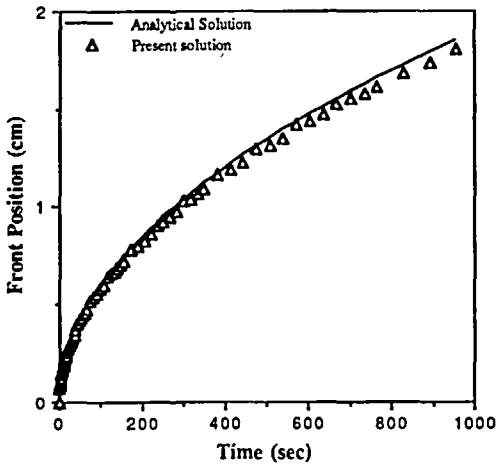

Figure 1 Front positions as a function of time in one-dimensional single phase change problem with water substance ($\Delta_{Tol}=8.0$ K)

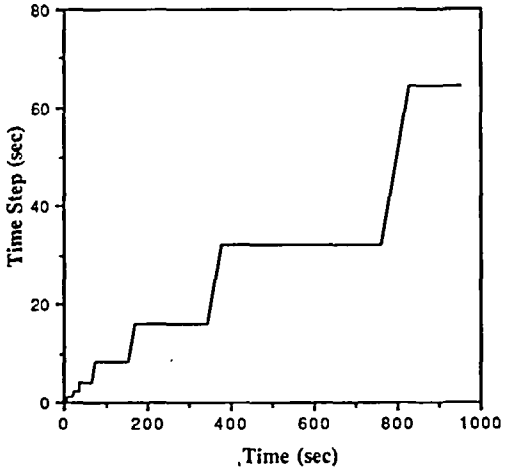

Figure 2 Time step history in one-dimensional single phase change problem ($\Delta_{Tol}=8.0$ K)

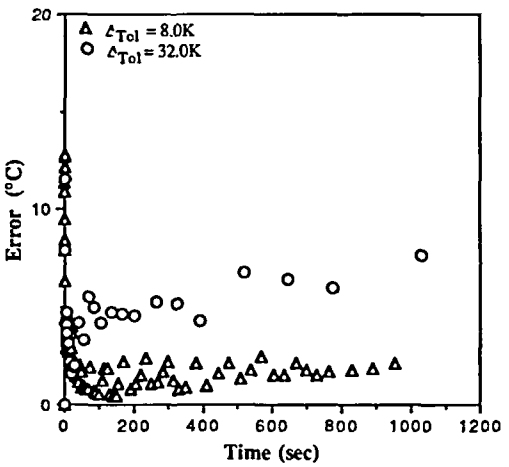

Figure 3 Maximum error history in one-dimensional solidification problem with water substance

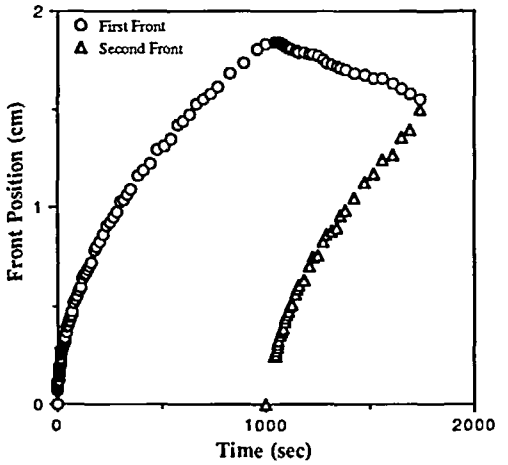

Figure 4 Front positions as a function of time in one-dimensional multiple phase change problem ($\Delta_{Tol}=$ 8.0 K)

problems require the time steps to adaptively adjust from small steps early in transient to increasingly large time steps to accurately monitor the exact solution. *Figure 3* shows the error histories of numerical results with initial tolerance $\Delta^0_{Tol}=8$ K and 32 K respectively, which also have been adaptively controlled. At the early stages the error is large since at $t\geqslant 0$, the boundary heat flux becomes infinite at $x=0$ [refer to (21)]. Also, one can see that the errors are significantly reduced by adaptively controlling the tolerance, Δ_{Tol}. This means that the time step is in good agreement with the theoretical predictions.

One-dimensional multiple phase change problem

In this example, solidification involving multiple phase fronts in a one-dimensional finite region $0\leqslant x\leqslant l$ is studied. The temperature boundary condition is applied at $x=0$ and an

adiabatic surface is assumed at $x=l$. Initially, the region is assumed liquid which is at a temperature higher than the melting temperature T_m. The material properties are given in *Table 1.*

The initial and boundary conditions for the example are as follows,

$$T(x, 0)=328.56 \text{ K}$$

$$T(0, t)=217.44 \text{ K} \qquad 0<t\leqslant 1000(\text{sec})$$
$$T(0, t)=328.56 \text{ K} \qquad 1000<t\leqslant 1800(\text{sec})$$

Twenty two-noded elements are used in this simulation and the length of the region $l=5.08$(cm). The integration parameter $\alpha=1$ in (10) is used.

Figure 4 gives the multiple phase front position history for the problem and *Figure 5* shows the adaptive time step history. The physics of the multiple existence of two phase fronts is evident from *Figure 4.* It is interesting to note that with the initiation of the second front, the first phase front starts traversing backward until the two phase fronts coalesce at a later time. It is also interesting to note that to account for changes in boundary conditions and temperature gradients, the time steps are adaptively adjusted and controlled to meet the adapted tolerance requirement.

Two-dimensional single phase change problem

In this example, solidification in an infinite corner region is studied. Initially, the region is assumed liquid which is at a temperature higher than the melting temperature T_m. The material properties are given in *Table 2.*

Table 2 Thermal properties

Heat conductivity in solid k_S	1.0 W/m-K
Heat conductivity in liquid k_L	1.0 W/m-K
Specific heat in solid c_S	1.0 J/kg-K
Specific heat in liquid c_L	1.0 J/kg-K
Density in solid ρ_S	1.0 kg/m^3
Density in liquid ρ_L	1.0 kg/m^3
Latent heat $\mathscr{L}$	0.25 J/kg
Melting temperature T_m	0.5°C

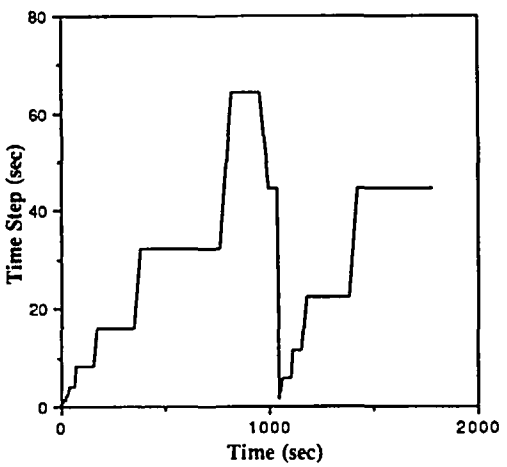

Figure 5 Time step history in one-dimensional multiple phase change problem. ($\Delta_{Tol}=8.0$ K)

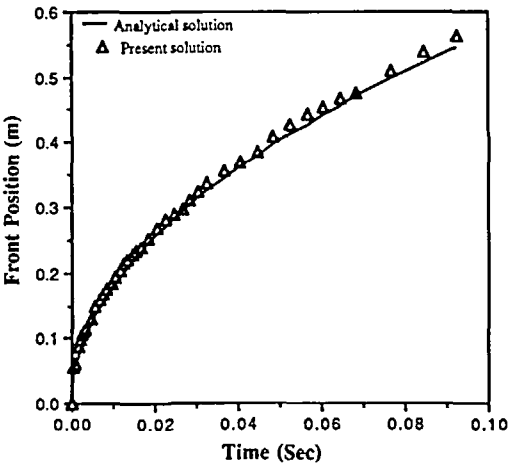

Figure 6 Front position along the diagonal line for solidification in an infinite corner region. ($\Delta_{Tol}=0.1$°C)

The initial and boundary conditions for the example are as follows,

$$T(x, y, 0)=0.3°C,\ T(0, y, t)=T(x, 0, t)=-1.0°C,\ T(\infty, \infty, t)=0.3°C$$

A total of 144 four-node elements and integration parameter $\alpha=0.5$ in (10) are used. The analytical solution and the non-dimensionalized interface position is given by Rathjen and Jiji[25],

$$y^*=\left[\lambda^u+\frac{C}{x^*-\lambda^u}\right]^{1/u} \tag{27}$$

where $C=0.159$, $u=5.02$, $l=0.70766$, $y^*=y/\sqrt{4at}$ and $x^*=x/\sqrt{4at}$, a $(=k/\rho c)$ is the thermal diffusivity ($a=1$ in this example). *Figures 6* and *7* give the comparative front positions along the diagonal line and $x=1.9$ (m) line, respectively. It can be seen that the present solution results agree well with the analytical solution. The adaptive time step history is shown in *Figure 8* for

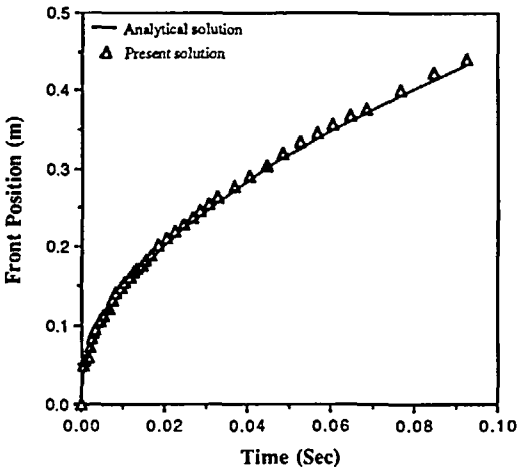

Figure 7 Front position along the $x=1.9$ (m) line for solidification in an infinite corner region. ($\Delta_{Tol}=0.1°C$)

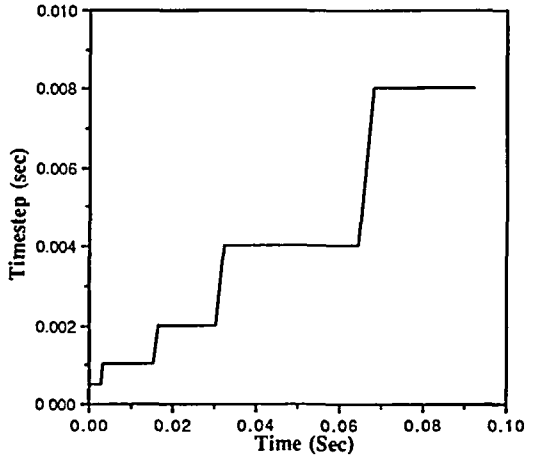

Figure 8 Time step history for solidification in an infinite corner region. ($\Delta_{Tol}=0.1°C$)

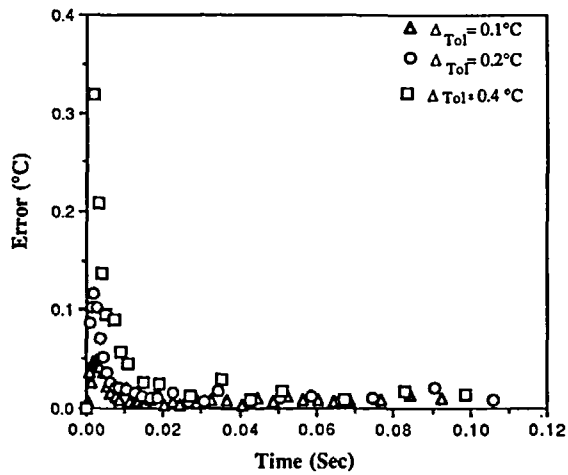

Figure 9 Maximum error history for solidification in an infinite corner region.

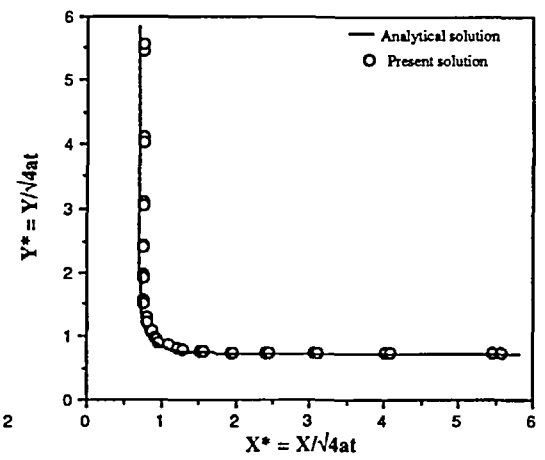

Figure 10 Non-dimensionalized front position for solidification in an infinite corner region. ($\Delta_{Tol}=0.1°C$)

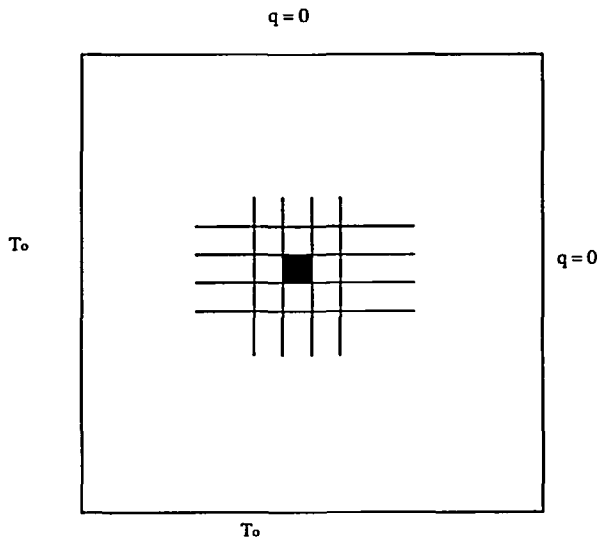

Figure 11 Description of two-dimensional geometry for two-dimensional multiple phase change problem

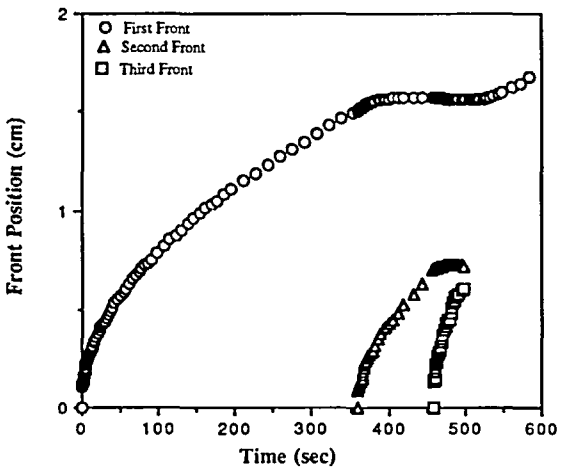

Figure 12 Front positions as a function of time along diagonal line for two-dimensional multiple phase change problem. (Water, $\Delta_{Tol} = 6.0$ K)

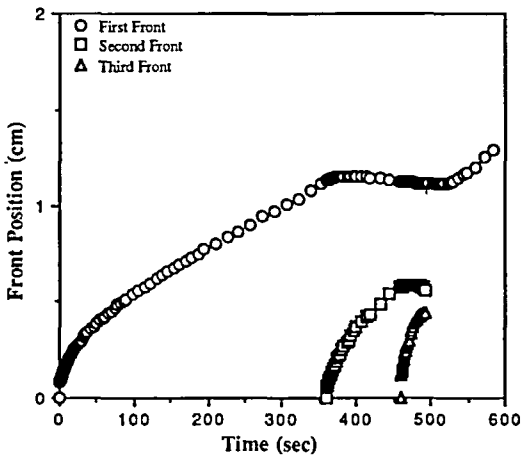

Figure 13 Front positions as a function of time along $x = 3.0$ (cm) line for two-dimensional multiple phase change problem. (Water, $\Delta_{Tol} = 6.0$ K)

$\Delta_{Tol} = 0.1$°C which was adaptively adjusted. The error histories for different tolerances are shown in *Figure 9* and it is clear that the errors can be controlled by adaptively adjusting the tolerances. The non-dimensional comparative front positions are given in *Figure 10* and are in excellent agreement with the analytical solution.

Two-dimensional multiple phase change problem

In this example, solidification involving multiple phases (co-existence of three phase fronts) in a finite corner region is studied. Initially, the region is assumed liquid which is at a temperature higher than the melting temperature T_m.

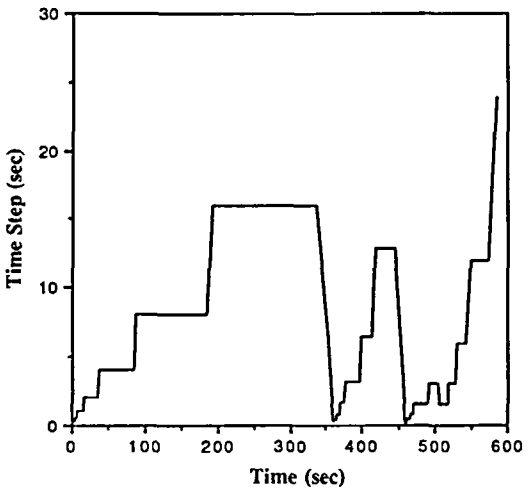

Figure 14 Time step history for two-dimensional multiple phase change problem. (Water, $\Delta_{Tol}=6.0$ K)

The initial and boundary conditions for the example are as follows,

$$T(x, y, 0)=328.56 \text{ K}$$
$$T(0, y, t)=T(x, 0, t)=217.44 \text{ K} \qquad 0<t\leqslant 350(\text{sec})$$
$$T(0, y, t)=T(x, 0, t)=300.78 \text{ K} \qquad 350<t\leqslant 460(\text{sec})$$
$$T(0, y, t)=T(x, 0, t)=217.44 \text{ K} \qquad 460<t(\text{sec})$$

The finite element model employed 400 four-node elements and the integration parameter $\alpha=1.0$ in (10) was used.

The material properties are given in *Table 1*. *Figure 11* shows the geometry of the square region. *Figures 12* and *13* show the front positions for the multiple phase change problem and *Figure 14* shows the adaptive time step history for this example.

It is interesting to observe the movement of the various phases, their interaction as time progresses and their behaviour (direction) when other phase fronts are initiated. The present problem clearly illustrates and provides a good understanding of the thermal behaviour and phase front interactions for two-dimensional regions.

From the above examples, it is clear that the adaptive time stepping approach is not only simple but is also efficient in controlling the global error in the simulation domain. The adaptive formulations are based on a posteriori error estimates leading to a reliable method and the numerical examples demonstrate the effectiveness and efficiency in controlling the global error.

CONCLUDING REMARKS

Solidification problems involving phase change with single or multiple co-existence of phases are described and have applications in many practical areas of engineering. The numerical simulations provided an accurate understanding of the thermal behaviour and phase front movements and interactions. The present simulations employed a robust adaptive time stepping strategy which is very cost-effective, especially for non-linear transient problems with phase change. The approach is very simple but yet is efficient and gives control of the global error for preserving solution accuracy.

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