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SHORT COMMUNICATION

A PHASE-CHANGE TEMPERATURE-BASED FORMULATION INCLUDING GENERAL LATENT HEAT EFFECTS

DIEGO CELENTANO AND EMILIO PÉREZ

E.T.S. d'Enginyers de Camins, Canals i Ports, International Center for Numerical Methods in Engineering (CIMNE), Universitat Politècnica de Catalunya, Gran Capità s/n, Mòdul C1, 08034 Barcelona, Spain

ABSTRACT

A phase-change temperature-based formulation including general latent heat effects is presented. These effects are taken into account by means of an explicit "phase-change function" (or liquid fraction-temperature relationship in a more specific context) defined analytically or based on experimental measurements. The behaviour of different functions is studied and compared. The finite element equations of this formulation are also described. Finally, a numerical example is analysed to illustrate the performance of the proposed methodology.

KEY WORDS Latent heat effects Phase-change problems

INTRODUCTION

Phase-change problems appear frequently in industrial processes and other problems of technological interest. The problem is highly non-linear owing to the latent heat effects and, therefore, few analytical solutions can be obtained[1]. Numerical solutions employing finite differences, boundary elements, or finite element techniques have been attempted by many researchers[2-5].

Among the finite element procedures, fixed domain methods have long been recognized to be the more suitable in dealing with general phase-change problems[2-5]. Within this framework, one option is to use the enthalpy as the main variable in order to take into account the latent heat effect. Once the enthalpy is known for each time step, the temperature can be obtained by means of the enthalpy-temperature relationship[2-7]. Other different approaches are the source method[8,9], transformation methods[10-12] and the transfinite element technique[13].

In particular, the enthalpy method has been coupled with a microscopic model of micro-structure formation during the solidification process[14]. In this model, the phase-change effects depend on several microscopic variables governing the kinetics phenomena. Another simplified macroscopic way to take these effects into account is by means of the definition of an explicit enthalpy-temperature relationship. This methodology has been used within the framework of the already mentioned methods[15-20]. Nevertheless, when the enthalpy-temperature relationship presents great variations or even discontinuities in the phase-change temperature range, all these

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methods need regularization in order to achieve convergence and stability of the numerical solution.

An alternative option, exploited first for thermal analysis[21] and more recently for thermal and general coupled thermomechanical formulations[22,23] consists of retaining the temperature as the only state variable of the thermal problem. In order to avoid any explicit smoothing, a special element able to integrate sharp or even discontinuous functions must be used[22,23]. Therefore, this methodology proves to be conservative in the weak form sense formulation satisfying the moving interface condition[22,23].

The objective of this paper is to present a phase-change model including general latent heat effects in the context of the temperature-based finite element formulation developed by Celentano *et al.*[22, 23]. In this new approach, all the advantages of the method presented in Celentano *et al.*[23] are preserved; that is, no regularizations on the phase-change function accounting for latent heat effects are required and convergent and stable numerical solutions are obtained. The governing equations of this problem are the energy equation with adequate boundary and initial conditions and a proper definition of the specific internal energy[22,23]. Some important details related to different analytical and experimental phase-change functions are discussed in the next section. The finite element formulation of this problem is then briefly described, and the final section includes a casting example of an Al-355 alloy where experimental results are compared with those obtained using the present formulation, showing in this form the effectiveness of the proposed methodology.

PHASE-CHANGE FUNCTION

In phase-change problems, the evolution of the specific internal energy ω is defined as[22,23]:

$$\dot{\omega} = c\,\dot{T} + L\,\dot{f}_{pc}\ , \tag{1}$$

where the superscript dot denotes time derivative, c is the specific heat capacity, T is the temperature, L is the specific latent heat released in a freezing problem (or absorbed in a melting one) and f_{pc} the "phase-change function". In the specific context of solidification problems related to a liquid to solid phase-change, the phase-change function is, in fact, the liquid fraction[22,23]. In this framework, the solid fraction f_s is defined as:

$$f_s = 1 - f_{pc}\ , \tag{2}$$

and constitutes a more usual variable in the experimental observations of solidification problems[15,16]. Equation (2) states that the choice of f_{pc} or f_s as the main variable that governs the phase-change phenomena is absolutely equivalent. Following Celentano *et al.*[22, 23], the first of them is adopted in this work.

For non-isothermal phase-change problems, f_{pc} can be written as[22,23]:

$$f_{pc}(T) = \begin{cases} 0 & ;\forall\, T \le \bar{T}_s \\ 0 < g(T) \le 1 & ;\bar{T}_s < \forall\, T \le \bar{T}_l \\ 1 & ;\forall\, T > \bar{T}_l. \end{cases} \tag{3}$$

where $\overline{T}_s$ and $\overline{T}_l$ denote the "solidus" and "liquidus" temperatures respectively while $g(T)$ denotes the way of latent heat release. Function $g(T)$ in equation (3) may be obtained using a microstructure model[14]. However, from a macroscopical point of view assumed in this paper, simpler choices for $g(T)$ can be adopted. In particular, the definition of several explicit bijective $g - T$ relationships have been attempted by different researchers[15-20]. Among them, it is possible to find:

- linear function

$$g(T) = (T - \bar{T}_s)/(\bar{T}_l - \bar{T}_s) \quad ;\forall\, \bar{T}_s < T \leq \bar{T}_l. \tag{4a}$$

- parabolic function:

$$g(T) = [(T - \bar{T}_s)/(\bar{T}_l - \bar{T}_s)]^2 \quad ;\forall\, \bar{T}_s < T \leq \bar{T}_l. \tag{4b}$$

- lever rule:

$$g(T) = 1 - (1/1 - k_p)\ [(T - \bar{T}_l)/(T - \bar{T}_m)] =$$

$$= [(\bar{T}_l - \bar{T}_m)/(T - \bar{T}_m)]\ [(T - \bar{T}_s)/(\bar{T}_l - \bar{T}_s)] \quad ;\forall\, \bar{T}_s < T \leq \bar{T}_l. \tag{4c}$$

where $k_p = (\overline{T}_l - \overline{T}_m)/(\overline{T}_s - \overline{T}_m)$ is the equilibrium partition ratio and $\overline{T}_m$ denotes the melting temperature of the pure metal matrix[15-20].

- function obtained experimentally: by means of the so-called cooling curve analysis[15,16] that consists, very briefly, of analysing the temperature evolution of a lumped-system (i.e. neglecting heat conduction) in order to know the $f_{pc} - T$ relationship. It should be emphasized that, although the values of f_{pc} are derived from the lumped-system assumption, they are only a function of casting temperature and, hence, applicable to modelling a general non-lumped casting solidification problem[15,16].

An example using these types of non-isothermal phase-change functions will be illustrated in the final section.

FINITE ELEMENT FORMULATION

In the context of the finite element technique[24], the discrete problem can be obtained via the spatial Galerkin projection of the continuous problem into a finite dimensional subspace ${}_hV$ of admissible C° continuous shape functions $N \in {}_hV$. Making use of the standard spatial interpolation for the temperature field, it leads to[24]:

$$\overset{t}{{}_h}T(\boldsymbol{x}) = \boldsymbol{N}(\boldsymbol{x})\ {}^t\boldsymbol{T}^{(e)}\ , \tag{5}$$

with $N_i \in {}_hV$ for $i = 1, \ldots, n_{node}$. In equation (5), N is the element shape function matrix and ${}^tT^{(e)}$ is the nodal temperature vector (the superscript e denotes element values). For simplicity in the notation, subscript h will be dropped from here onwards.

Following standard procedures, the global discretized thermal equilibrium equations at a certain time can be written in matrix form as[22,23]:

$$\boldsymbol{R} = \boldsymbol{F} - \boldsymbol{C}\,\dot{\boldsymbol{T}} - \boldsymbol{K}\,\boldsymbol{T} - \dot{\boldsymbol{L}} = \boldsymbol{0}\ , \tag{6}$$

where F is the external heat flux vector, C is the capacity matrix, K is the conductivity matrix, L is the "phase-change" vector rate and R is the residual vector[22,23]. As usual, all vectors and matrices are assembled from the element contributions in the standard manner[24]. The form of the different elemental expressions appearing in equation (6) can be seen in Celentano *et al.*[22,23]. However, it is important to remark that the elemental contribution of L is[22,23]:

$$\dot{\boldsymbol{L}}^{(e)} = \int_{\Omega^{(e)}} \boldsymbol{N}^{\mathcal{T}}\ \rho_o\ L\ \dot{f}_{pc}\ d\Omega\ , \tag{7}$$

where ρ_0 is the density at the reference configuration of body Ω and $\mathcal{T}$ is the transpose symbol. Also it should be noted that the term $\dot{L}$ contains the latent heat effect when $\dot{f}_{pc} \neq 0$.

To integrate in time equation (6), a generalized mid-point rule algorithm can be used[24]. In particular, the well-known Euler backward method has been used in this work.

As f_{pc} can present sharp variations or jump discontinuities inside an element in the presence of phase-change, a non-standard spatial integration is needed to compute L accurately. The idea used in this paper consists of splitting the $\Omega^{(e)}$ integral into $\Omega^{(e)}_{n_{div}}$ integrals, with the number of element

subdivisions n_{div} fixed. Using this subdomain technique, a more accurate integration is achieved[22,23].

Finally, particular details concerning the solution strategy algorithm for solving the non-linear system of equation (6) can be found in Celentano *et al.*[22,23].

NUMERICAL EXAMPLE

Solidification of an Al-355 alloy

Some experiments using an Al-355 alloy with a sand mould have been conducted by Su and Tsai[15] in order to obtain the phase-change function f_{pc} during the solidification process. To this end, several very sensitive thermocouples were used for temperature measurements. The thermophysical properties of this problem have been reported in Su and Tsai[15] and they can be found in the following:

Thermal properties of aluminium Al-355

- Density: $\rho_0 = 2{,}710\left[\frac{K_g}{m^3}\right]$
- Specific heat capacity: $c = 963\left[\frac{J}{KgK}\right]$
- Conductivity coefficient: $k = 160\left[\frac{J}{msK}\right]$
- Solidus temperature: $\overline{T}_s = 818[K]$
- Liquidus temperature: $\overline{T}_l = 893[K]$
- Melting temperature of pure aluminium: $\overline{T}_m = 933[K]$
- Latent heat: $L = 389{,}000\left[\frac{J}{kg}\right]$

Thermal properties of moulding sand

- Density: $\rho_0 = 1{,}730\left[\frac{K_g}{m^3}\right]$
- Specific heat capacity: $c = 547 + 1.146T - 5.4 \times 10^{-4}T^2\left[\frac{J}{KgK}\right]$
- Conductivity coefficient: $k = 0.604 - 0.767 \times 10^{-3}T + 0.795 \times 10^{-6}T^2\left[\frac{J}{msK}\right]$

Thermal properties of the interfaces

- Convection-radiation coefficient (sand-air): $h = 90\left[\frac{J}{m^2sK}\right]$
- Environmental temperature: $T_{env} = 298.16[K]$
- Convection-radiation coefficient (aluminium-sand): $h_g = 300\left[\frac{J}{m^2sK}\right]$

The numerical analysis begins with the mould completely filled with aluminium in liquid state. The initial temperatures are supposed to be $950K$ for the casting and $298.16K$ for the mould.

The geometry, boundary conditions and 2D plane finite element mesh used in the computations are presented in Figure 1. The time step chosen was $\Delta t = 5\ s$.

Figure 2 shows the different phase-change functions considered in the numerical analysis. The experimental phase-change function has been obtained in Su and Tsai[15]. In sharp contrast with Su and Tsai[15] and Jong and Hwang[16], it should be noted that no regularization has been performed on this curve because, as mentioned before, the formulation presented in the previous section is able to deal with this kind of function.

The temperature evolution of two points situated in the alloy are plotted in Figures 3 and 4 respectively, where it is clearly seen that the lumped-system condition is fulfilled, as it has been pointed out in Su and Tsai[15]. These cooling curves show that the Al-355 alloy is characterized by two "plateaux" corresponding to peaks of latent heat release. The shapes of such curves represent a typical trend for many hipoeutectic alloys[15,16]. It should be noted that a very good agreement between numerical results using the experimental phase-change function and experimental measurements is achieved. On the other hand, a significant difference in temperature history for the linear function was found. Moreover, the parabolic and lever functions do not predict the two flat segments but they behave reasonably well in the whole solidification range. Therefore, the selection of correct mode of latent heat release during solidification is crucial to predict the temperature distribution and solidification pattern in castings.

Finally, Figure 5 depicts the temperature history at a point located in the external surface of the mould.

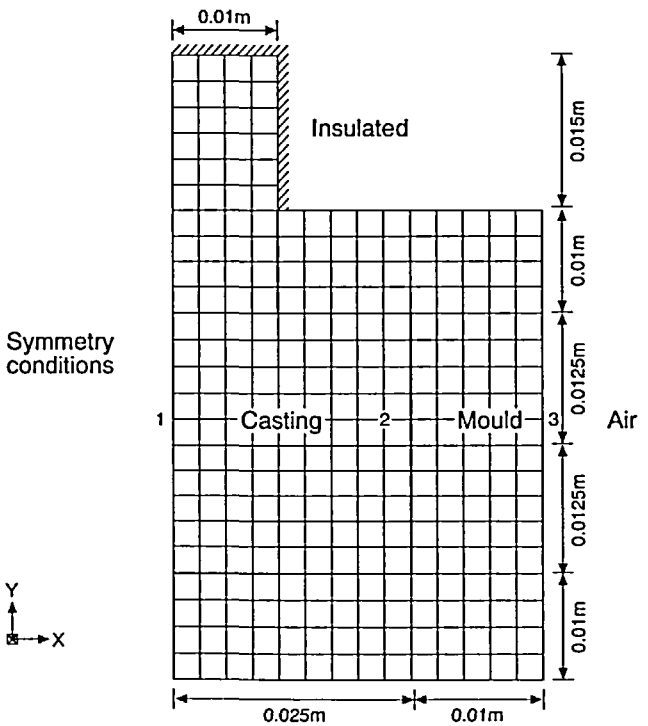

Figure 1 Geometry, boundary conditions and finite element mesh (four-noded elements)

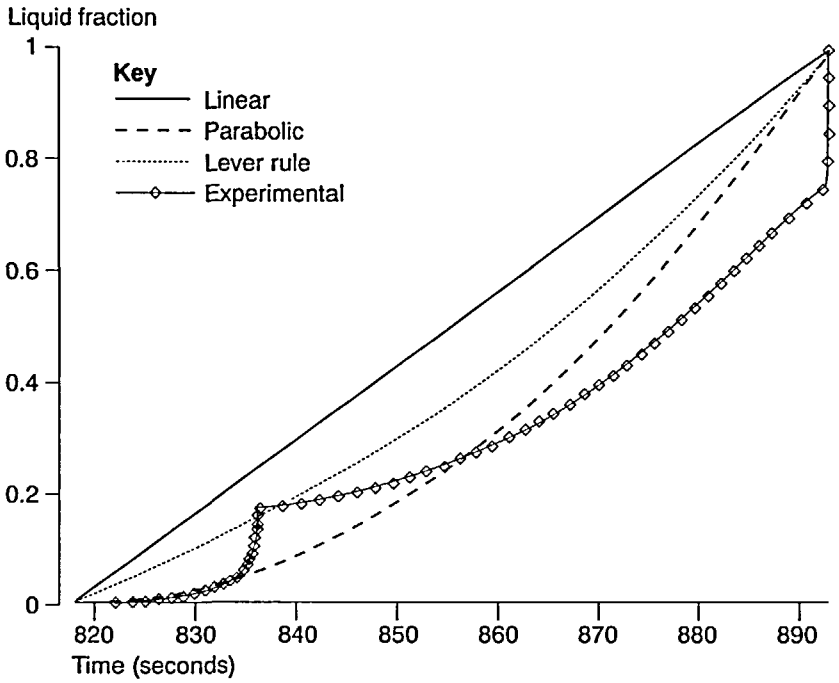

Figure 2 Phase-change functions

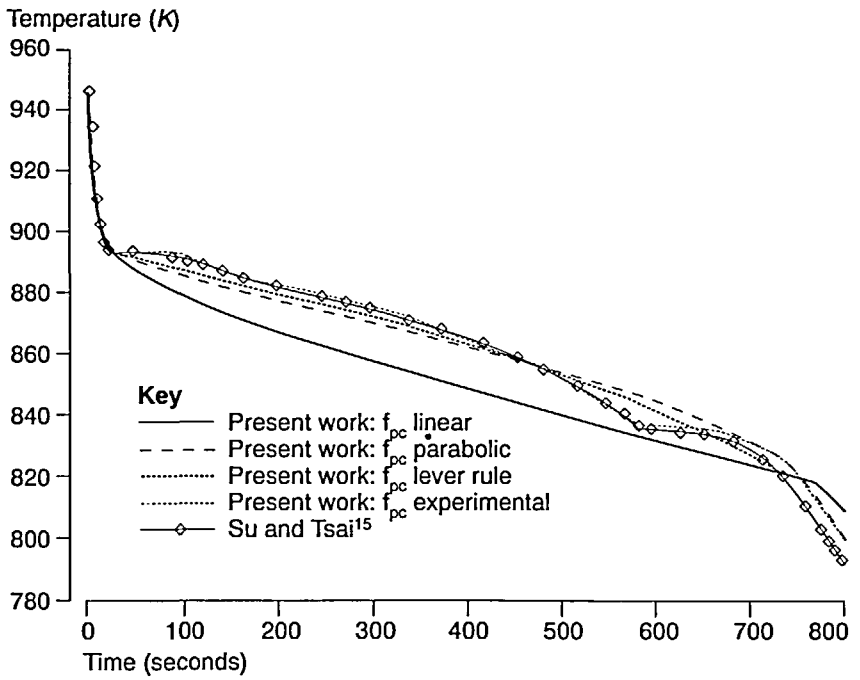

Figure 3 Temperature evolution at point 1

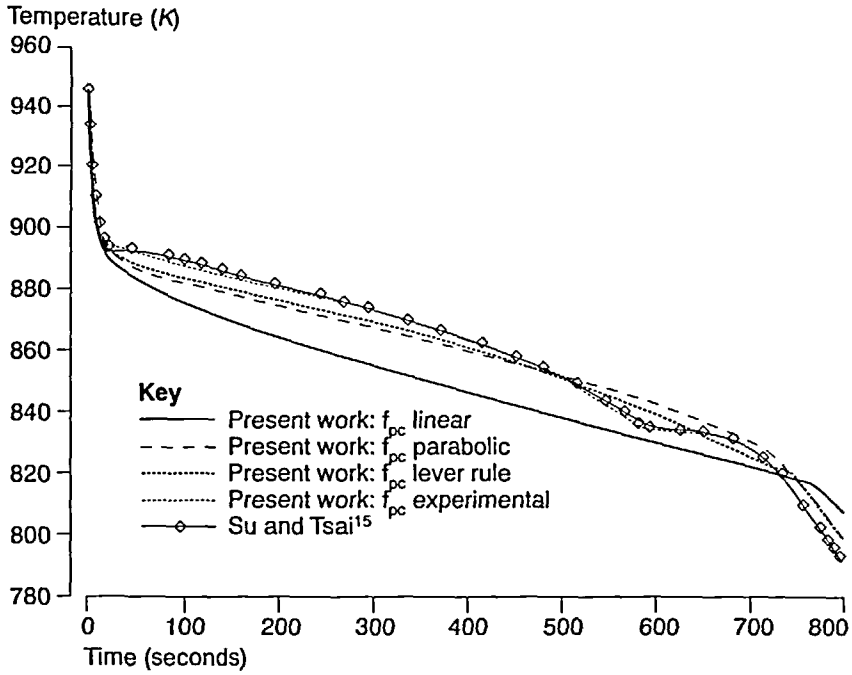

Figure 4 Temperature evolution at point 2

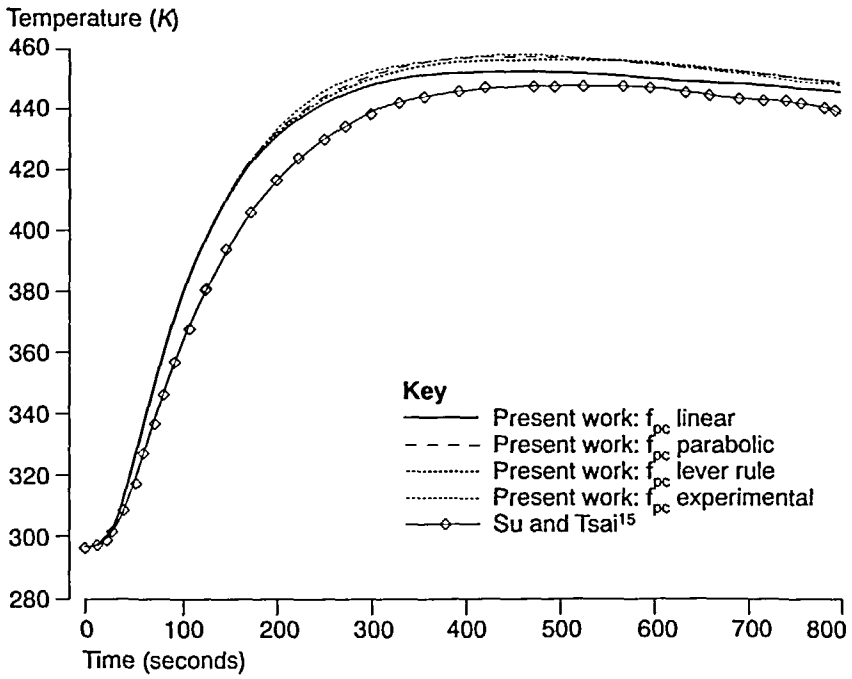

Figure 5 Temperature evolution at point 3

CONCLUSIONS

A temperature-based finite element formulation able to deal with general latent heat effects has been presented. The main features of such a formulation are:

- it can solve generalized phase-change problems taking into account general latent heat effects;
- it does not need any explicit regularization on the phase-change function because an accurate integration technique is employed. Thus, it is conservative in the weak form sense;
- the numerical example analysed shows the accuracy of the present formulation. In particular, an appropriate experimental-based mode of latent heat release is required for correctly modelling real casting solidification problems.

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