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ENTHALPY GRADIENT METHODS FOR CAPTURING LATENT HEAT IN PHASE CHANGE SIMULATIONS USING BIQUADRATIC ISOPARAMETRIC FINITE ELEMENTS

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ABSTRACT

Methods that use spatial gradients of enthalpy to evaluate effective specific heats and capture latent heat effects in phase change problems have been used successfully in finite element formulations based on linear interpolation. In view of the greater geometrical flexibility and efficiency of biquadratic isoparametric elements, it is of interest to assess the use of the methods with these elements. In comparisons with an accurate semi-analytic solution for a test problem, it is shown that the enthalpy gradient methods with quadratic interpolation are prone to error. A new procedure is proposed that uses bilinear sub-elements for enthalpy, formed by subdivision of the biquadratic temperature elements. This is shown to be accurate and robust, for phase change intervals as small as 0.02°C.

KEY WORDS Phase change Latent heat Enthalpy gradient methods

THE EFFECTIVE SPECIFIC HEAT METHOD FOR MELTING AND SOLIDIFICATION

A popular and generally successful method for treating latent heat effects in phase change is by the use of an effective specific heat, C_{eff}, as illustrated in *Figure 1*. Here, the latent heat is distributed over a more or less narrow temperature range, and appears as a peak in the plot of effective specific heat *versus* temperature. The method is computationally convenient, because the heat transfer in both phases can be solved as a single problem, without the need to track the interface explicitly. It can also be generalised to multidimensions in a straightforward way, and existing heat transfer codes can be adapted to include phase change, by adding a subroutine to define a temperature dependent effective specific heat, $C_{eff}(T)$, as in *Figure 1a*, along with other temperature dependent physical properties.

Difficulties can arise, though, in using this approach. In treating pure materials, which have sharply defined melting points, the physics must be approximated by spreading latent heat effects over at least a narrow temperature interval. Potentially more serious, though, than this physical approximation is the possibility that the peak in effective specific heat may be 'skipped' in the computations if $C_{eff}(T)$ is obtained in the straightforward way described above. This can occur if the phase change falls entirely between integration points, or within a time step. In dealing with more complex materials, such as alloys or semi-crystalline polymers, the phase change does, in fact, extend over a significant temperature range, and traces from differential scanning calorimetry can show peaks in effective specific heat that may have a base width of 10 or 20°C.

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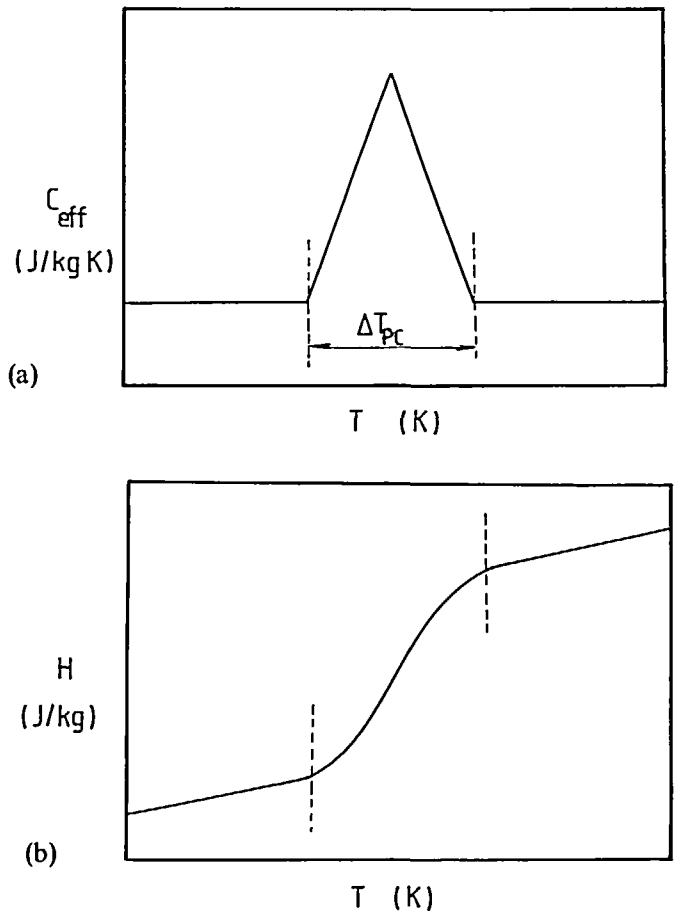

Figure 1 (a) The effective specific heat, C_{eff}, as a function of temperature. The area under the peak represents the latent heat of phase change. $C_{eff}(T)$ is idealized here by piecewise linear functions. (b) The corresponding plot of enthalpy, H, as a function of temperature

The danger of skipping the peak is then reduced, but the physics is still approximated, because the position and width of the peak can depend on scanning rate and on whether heating or cooling is used. In a practical problem, a range of heating or cooling rates will occur, and no particular DSC trace will be entirely appropriate. The only way of avoiding this difficulty is to obtain latent heat effects by modelling the crystallization kinetics, coupled with the heat transfer. However, in view of the complexity of this undertaking, it is clear that techniques such as the effective specific heat method will continue to be used.

Techniques designed to avoid latent heat 'skipping' have been proposed in the finite element literature, based on the use of enthalpy, H, which is related to the effective specific heat, C_{eff} by:

$$H(T) = \int_{T_{datum}}^{T} \rho C_{eff}\, dT' \tag{1a}$$

hence:

$$\frac{dH}{dT} = \rho C_{eff} \tag{1b}$$

Figure 1b illustrates this function of temperature. The basic idea is to utilize enthalpy differences over finite intervals of time or space. Spatial differencing has been more widely used, and is the subject of the present note. From a subroutine defining the function $H(T)$, enthalpy values are assigned to nodes consistent with the current temperature solution. Enthalpy is interpolated within elements using the same shape functions as for temperature, and values of ρC_{eff} calculated at integration points using spatial gradients of temperature and ehthalpy. Thus, Comini *et al.*[1] proposed:

$$C_{\text{eff}} = \frac{1}{3}\left[\frac{\partial H/\partial x}{\partial T/\partial x} + \frac{\partial H/\partial y}{\partial T/\partial y} + \frac{\partial H/\partial z}{\partial T/\partial z}\right] \tag{2}$$

for use with linear triangular elements.

In subsequent work del Guidice, Comini and Lewis[2] used derivatives in the direction, s, of the temperature gradient:

$$\frac{\partial H}{\partial T} = \frac{\partial H/\partial s}{\partial T/\partial s} \tag{3a}$$

hence in two dimensions:

$$\rho C_{\text{eff}} = \frac{\left(\dfrac{\partial H}{\partial x}\dfrac{\partial T}{\partial x} + \dfrac{\partial H}{\partial y}\dfrac{\partial T}{\partial y}\right)}{\left[\left(\dfrac{\partial T}{\partial x}\right)^2 + \left(\dfrac{\partial T}{\partial y}\right)^2\right]} \tag{3b}$$

and applied this using biquadratic isoparametric elements. Lemmon[3] gave a detailed exposition of the use of spatial gradients, showing how, for linear interpolation, a true mean value of ρC_{eff} over the element is obtained and proposed:

$$\rho C_{\text{eff}} = \left[\frac{\left(\dfrac{\partial H}{\partial x}\right)^2 + \left(\dfrac{\partial H}{\partial y}\right)^2}{\left(\dfrac{\partial T}{\partial x}\right)^2 + \left(\dfrac{\partial T}{\partial y}\right)^2}\right]^{1/2} \tag{4}$$

for use in two dimensions.

Thomas, Samarsekera and Brimacombe[4] in a comparison of the del Guidice, equation (3b), and Lemmon, equation (4), methods with linear triangular elements, found that the Lemmon formula gave slightly better results. Regarding element type they remarked that 'the discontinuous temperature field across the solid–liquid boundary would be better approximated by a large number of elements than by a few higher order elements'. It is, of course, the temperature gradient that is discontinuous across the phase boundary, and this only when the melting point is sharply defined. The assertion that linear elements are better for phase change problems was, however, repeated by Dalhuijsen and Segal[5], who found both the Lemmon and del Guidice methods satisfactory, and superior to ones based on fictitious heat flow. The difficulty in computing phase change arises from the sharp changes in effective specific heat, and enthalpy, rather than from discontinuities in temperature gradient. Provided that reliable mean values of effective specific heat can be obtained at integration points, the use of higher order elements is attractive, for all the usual reasons of efficiency and geometrical flexibility. The spatial averaging techniques reviewed above were originally proposed for linear elements, where it is clear that true element mean values are given. The key question, and the subject of the present work, is whether and how they can be extended to higher order elements. Despite their apparently successful use with biquadratic isoparametric elements by del Guidice *et al.*[2], it turns out that their straightforward use can lead to errors.

In the following we test the del Guidice and Lemmon methods on biquadratic isoparametric elements in a solidification problem with a known solution. Having identified the source of errors, a technique is proposed that overcomes the difficulty and efficiently provides results of high accuracy.

TEST PROBLEM

We compare our numerical solutions with a result obtained by Rathjen and Jiji[6], which, though it includes some approximations, is believed to be of high accuracy. These authors considered cooling and solidification of material in the symmetric corner, $x, y > 0$, initially liquid at temperature T_i, greater than or equal to the sharply defined freezing temperature, T_F. At time $t \geqslant 0$, the boundaries $x = 0$, $y = 0$ are reduced to and maintained at T_w, $T_w < T_F$. The densities of both phases are taken to be equal, as are the thermal diffusivities. The problem was solved by superimposing solutions corresponding to a simple conduction problem, and one involving a moving heat source representing the latent heat release at the interface. The shape of the interface is fitted (approximately) by a superhyperbola with two adjustable parameters λ and m. λ is obtained as a function of β, the latent to sensible heat ratio, from a plot supplied in their paper; x_0^* and x_1^*, two dimensionless lengths, are also read from plots against β. m is then found from the a further plot as a function of x_0^*/λ and x_1^*/λ. We outline this procedure here because the accuracy of reading these various plots is limited, and it is important to assess the size of possible errors on the solution values that result. A further parameter to be chosen in the evaluation of the solution is Λ, introduced to eliminate an infinite limit in a quadrature, which is carried out using Gauss' method, with 40 points in each coordinate direction. The resulting expression is rather cumbersome and is not reproduced here. Rathjen and Jiji assess the accuracy of their results by comparison with a finite difference solution. Differences are generally about 0.15% of $(T_i - T_w)$, the imposed temperature change. Part of the discrepancy may, of course, be due to truncation errors in the finite difference solution. The present calculations were carried out with initial and boundary conditions (dimensions m, see *Figure 2*):

$$
\begin{array}{llll}
t < 0 & 0 \leqslant x \leqslant 0.762 & 0 < y \leqslant 0.762 & T = T_i = 1535°\text{C} \\
t \geqslant 0 & x = 0 & 0 < y \leqslant 0.762 & T = T_w = 1150°\text{C} \\
 & y = 0 & 0 < x \leqslant 0.762 & T = T_w = 1150°\text{C} \\
 & \text{x} = 0.762 & 0 < y \leqslant 0.762 & \dfrac{\partial T}{\partial x} = 0 \\
 & y = 0.762 & 0 < x \leqslant 0.762 & \dfrac{\partial T}{\partial y} = 0
\end{array}
$$

and physical properties:

Solidification temperature	$T_F = 1500°\text{C}$
Thermal conductivity	$k = 30\ \text{W/m}\ °\text{C}$
Density	$\rho = 7200\ \text{kg/m}^3$
Specific heat	$C = 750\ \text{J/kg}\ °\text{C}$
Latent heat of fusion	$L = 262.5 \times 10^3\ \text{J/kg}\ °\text{C}$

giving

$$\beta = \frac{L}{C(T_F - T_W)} = 1.0, \qquad T_i^* = \frac{T_i - T_F}{T_F - T_W} = 0.1$$

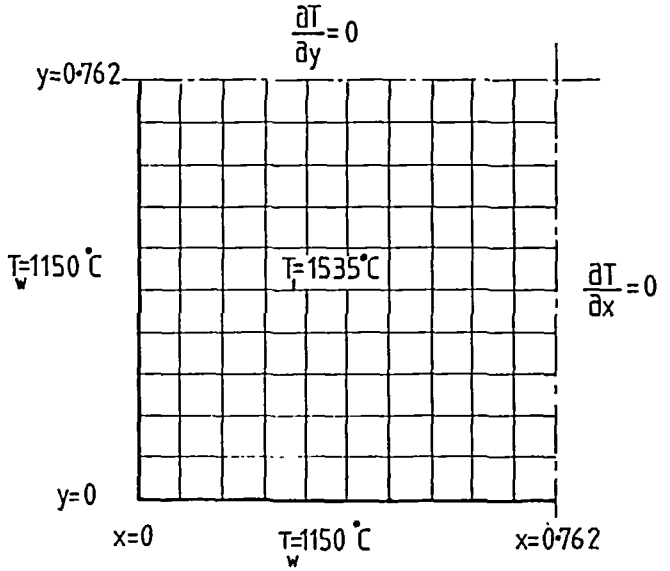

Figure 2 The domain and initial and boundary conditions of the test problem. The mesh of biquadratic Lagrangian elements is also shown

Note that ρ, k and C are taken to be the same in both liquid and solid phases. Reading from the plots provided by Rathjen and Jiji[6]

$$x_0^* = 0.680 \pm 0.002$$
$$x_1^* = 0.770 \pm 0.002$$
$$\lambda = 0.580 \pm 0.002$$

leading to

$$\frac{x_0^*}{\lambda} = 1724 \pm 0.0075 \qquad \frac{x_1^*}{\lambda} = 1.3280 \pm 0.0080$$

Reading m as a function of these values we find $2.5 \leqslant m \leqslant 4.5$, approximately. The uncertainty in m seems rather large, but fortunately the solution is insensitive to this. Calculation of the temperature at, for example, $x = y = 0.1905$ m, and $t = 5400$ s gives $T = 1388.5 \pm 0.1$°C; i.e. the resulting uncertainty in T is about 0.03% of the imposed temperature difference $(T_i - T_W)$. Finally, we comment on the choice of the parameter Λ. Rathjen and Jiji suggest $\Lambda > 3\lambda$, or if $T_i^* > 1.0$ and $\beta > 1.0$, then $\Lambda > 5\lambda$ is required. Consistent with this our numerical experiments showed the solution to be independent of Λ for $\Lambda > 4\lambda$, which value was used in the results reported.

It therefore seems likely that results derived from the Rathjen and Jiji paper are accurate to better than 0.15% of $(T_i - T_W)$ or 0.6°C in the present test problem. It is therefore meaningful to make comparisons with the finite element results at this level.

FINITE ELEMENT SOLUTIONS

The domain of the test problem was discretized using a regular 11 × 11 mesh of isoparametric biquadratic Lagrangian elements, *Figure 2*. Finite element equations were formed in the usual

way, using the Galerkin procedure, with the θ-method for time-stepping. The equations were linearized by evaluating the specific heat, $\mathbf{M}^n$, and conductivity, $\mathbf{K}^n$, matrices corresponding to temperature T^n, at the start of the time step:

$$M^n\left(\frac{\mathbf{T}^{n+1}-\mathbf{T}^n}{\Delta t}\right)+\mathbf{K}^n[(1-\theta)\mathbf{T}^n+\theta\mathbf{T}^{n+1}]=\mathbf{f}^n \tag{5}$$

θ was chosen as 0.75 to give a balance between stability and lack of oscillations, and truncation error. Mass lumping of $\mathbf{M}$ was not applied, as numerical experiments showed that lumping gave less accurate results. Introduction of the step change in the surface temperature at $t = 0$ injects oscillations into the numerical solution, which, though they die away, are undesirable. The numerical solution was therefore started from $t = 480$ s, using as initial conditions values obtained from the Rathjen and Jiji theory, which, of course, incorporate the required boundary conditions at $x = 0, 0 < y \leqslant 0.762$ m; $y = 0, 0 < x \leqslant 0.762$ m. Zero normal temperature gradient conditions were applied in the usual way at the internal boundaries $x = 0.762$ m, $0 < y \leqslant 0.762$ m; $y = 0.762$ m, $0 < x \leqslant 0.762$ m. The time step was set at 120 s, and the solutions run to 5400 s. At this time the dimensionless distances x^* and y^* [$x^* = x/(\sqrt{4\alpha t})$, α = thermal diffusivity] corresponding to the internal boundaries are approximately equal to Λ, as required: that is, the solution near the boundaries is effectively 1-dimensional, justifying the use of the zero normal heat flux boundary condition.

The effective specific heat was represented in a subroutine using piecewise continuous linear functions of temperature, as illustrated in *Figure 1a*; and enthalpy correspondingly, with quadratic functions in the phase change interval, *Figure 1b*. In a series of runs this interval ΔT_{PC} (the base width of the effective specific heat peak) was taken as 0.02°C, 0.2°C, 2°C, 5°C, 10°C, 20°C and 30°C, whilst maintaining the latent heat constant.

Results are examined at nodes on the diagonal $x = y$, for $0 < x \leqslant 0.381$ m, which spans the region affected by the phase change throughout the simulation. The percentage departure of a computed nodal value, T_c, from the theoretical value, T_t, is defined as

$$e=\frac{T_c-T_t}{T_i-T_W}\times 100\%$$

and the mean error over the 11 nodes is

$$\bar{e}=\frac{\sum_{n=1}^{11}|e_n|}{11}$$

Figures 3a and *3b* show values of $\bar{e}$ obtained at $t = 2400$ s and $t = 5400$ s using:

(i) The direct effective specific heat method, with integration point values obtained directly from $C_{\text{eff}}(T)$.
(ii) The del Guidice method, equation (3b).
(iii) The Lemmon method, equation (4).

In (ii) and (iii) integration point values of the spatial gradients of enthalpy are obtained from the biquadratic interpolation of this quantity.

The figures show, as expected, that the direct effective specific method fails badly for small phase change intervals, giving an error of 13% for $\Delta T_{PC} = 2$°C at $t = 5400$ s. Only when $\Delta T_{PC} \approx 30$°C do the results approach those obtained using the del Guidice and Lemmon methods. At $t = 2400$ s these show very similar errors of about 1%, constant over the whole range of ΔT_{PC}. However, at $t = 5400$ s less simple behaviour is observed; errors for the Lemmon method are again around 1% over the whole range, but the del Guidice results show irregular behaviour as ΔT_{PC} is reduced, with errors up to 9%. In view of the apparent similarity of the methods, this may initially seem surprising. The explanation, though, is not hard to find. For small ΔT_{PC},

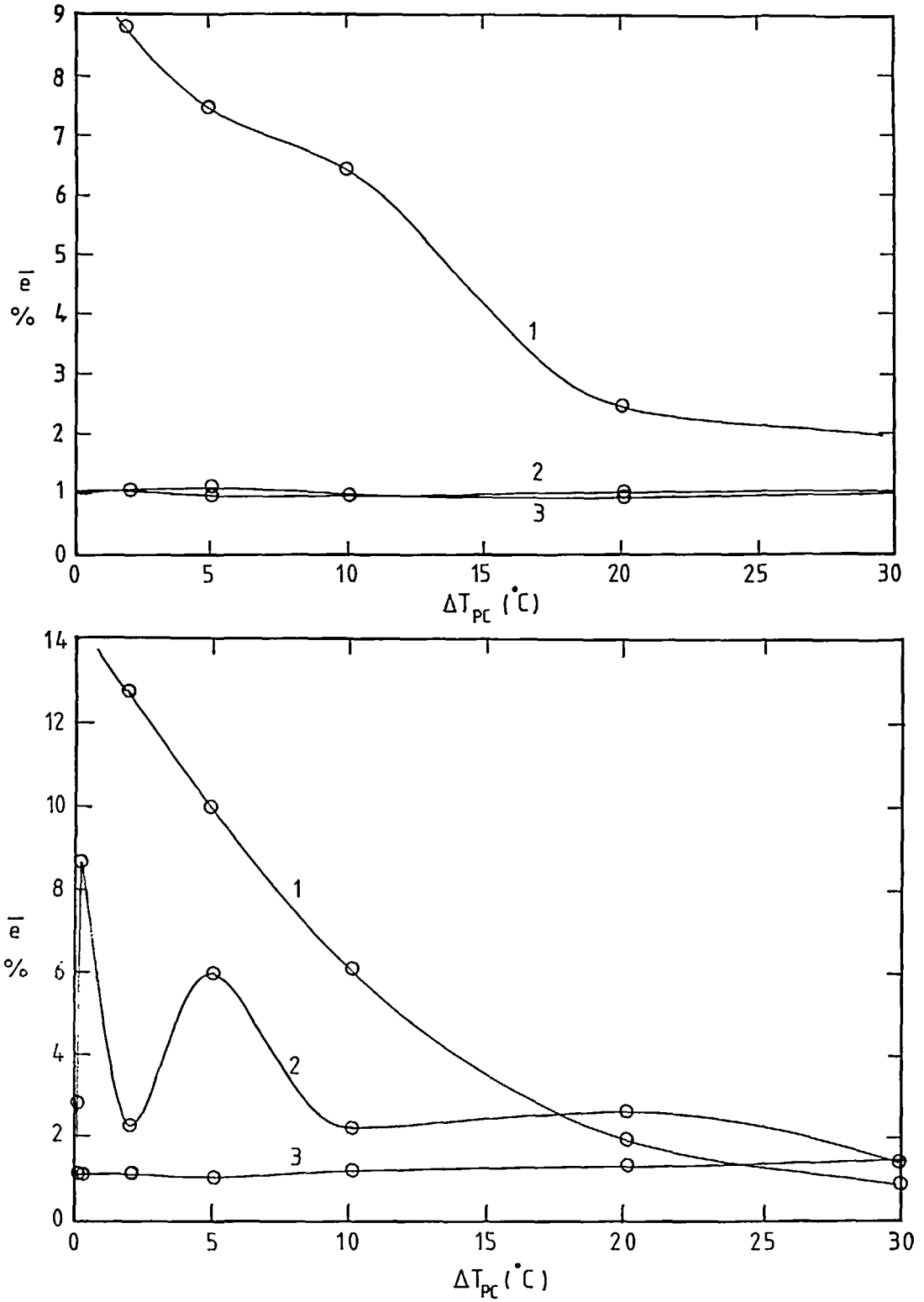

Figure 3 Mean departures, $\bar{e}$, of the computed from the theoretical temperatures in the test problem. Computational method for latent heat: (i) direct use of effective specific heat; (ii) del Guidice method, equation (3b); (iii) Lemmon method, equation (4). (a) (upper plot) Cooling time $t = 2400$ s; (b) (lower plot) $t = 5400$ s

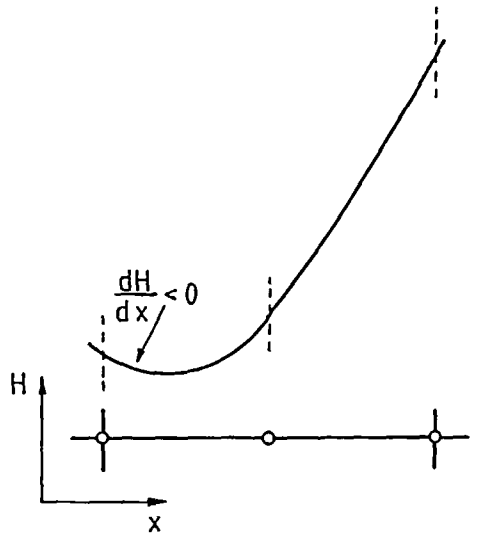

Figure 4 Illustration of the failure of quadratic interpolation of enthalpy to provide correct spatial derivatives in a phase change region

where nodal enthalpy values change sharply within an element, the biquadratic interpolation is unable to provide reliable integration point values of the spatial derivatives. This is illustrated in *Figure 4*, from which it is clear that incorrect negative gradients may occur. The effect of these is masked in the Lemmon formula, because squares of gradients are used; hence its rather better performance. Nevertheless, incorrect values of C_{eff} are produced.

It is clear, then, that the methods based on enthalpy gradients are unsatisfactory when quadratic (or higher order) interpolation is used. We are reluctant, though, to forgo the advantages of biquadratic isoparametric elements in representing temperature fields (and velocity fields in coupled problems). We therefore propose the procedure described in the following section.

BILINEAR SUB-ELEMENTS FOR ENTHALPY

At each time step, nodal temperatures are scanned, to establish which elements are affected by phase change. In those that are not, specific heat is obtained in the straightforward way as a function of temperature at the 3 × 3 integration points. Phase change elements, however, are subdivided into four bilinear sub-elements, as shown in *Figure 5*. The sub-elements are then

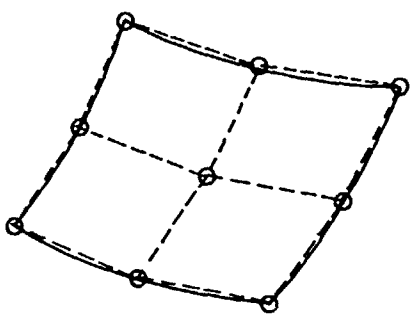

Figure 5 Subdivision of an isoparametric biquadratic Lagrangian element into four bilinear sub-elements

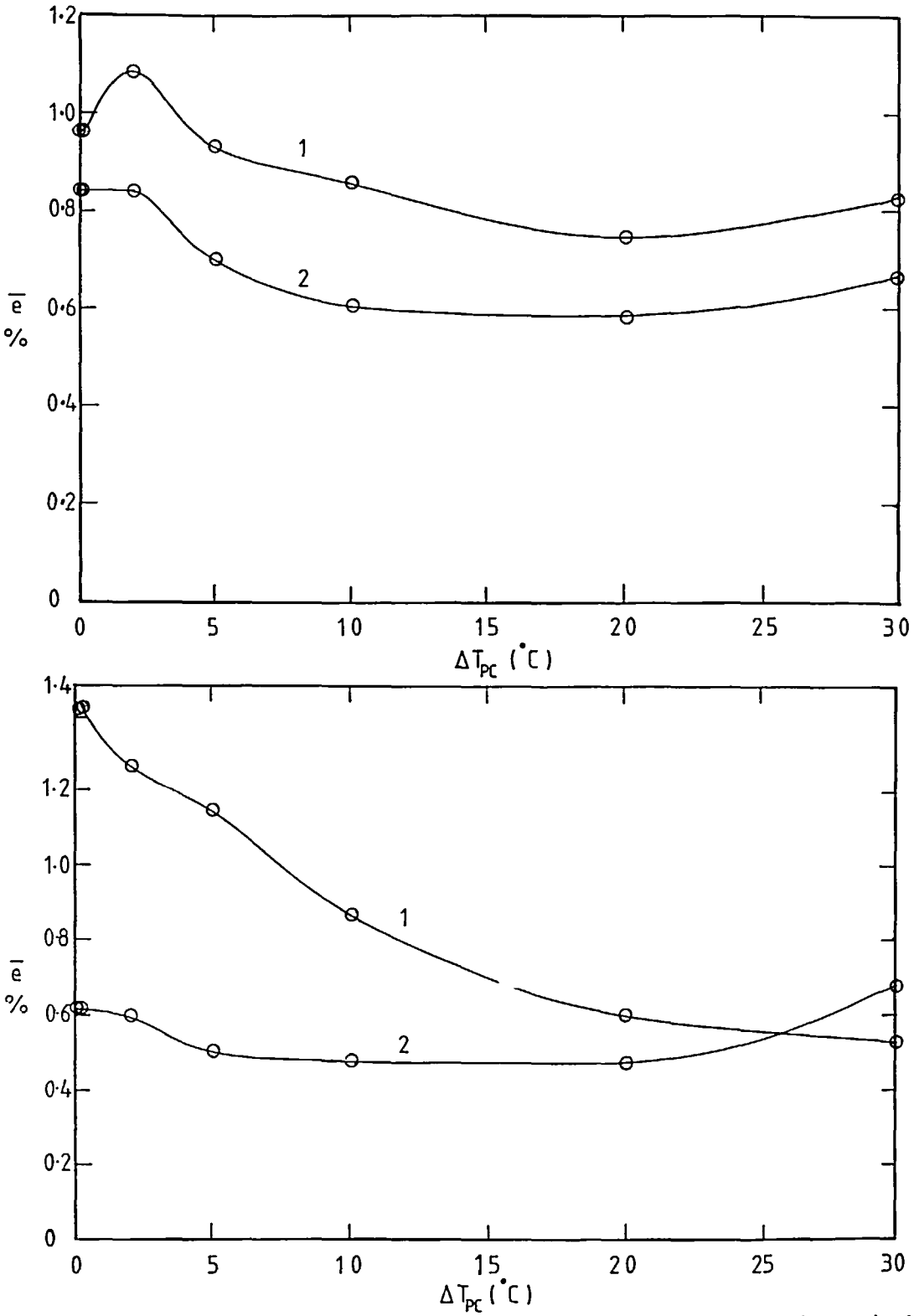

Figure 6 Mean departure, $\bar{e}$, of the computed from the theoretical temperatures in the test problem. Computational method: revised algorithm using bilinear sub-elements. (i) the del Guidice method; (ii) the Lemmon method. (a) (upper plot) Cooling time $t = 2400$ s; (b) (lower plot) $t = 5400$ s

scanned, and, in those unaffected by phase change, specific heat is again obtained straightforwardly at the 2 × 2 integration points. In sub-elements affected by phase change, the del Guidice or Lemmon methods are used, based on spatial gradients from bilinear interpolation of enthalpy. Contributions from the sub-elements are assembled into the stiffness matrix for the parent biquadratic element, and the solution is completed as usual.

This procedure avoids the false gradient values that can arise from quadratic interpolation of enthalpy, whilst retaining the advantages of higher order isoparametric elements in representing the temperature field. It could be regarded as a simple form of dynamic adaptive mesh refinement for phase change, and can obviously be extended to further levels of subdivision of the biquadratic elements, if this should prove necessary. Computing costs are increased by the use of 16 rather than 9 integration points, but only in those elements where phase change is occurring, and this seems a small price to pay for proper handling of the latent heat.

The test problem was re-run using the procedure described, and results are shown in *Figure 6*. At $t = 2400$ s, mean errors, $\bar{e}$, in the computed results are generally below 1%; at $t = 5400$ s the del Guidice method produces errors up to 1.4% for small ΔT_{PC}, whilst for the Lemmon method errors are around 0.6%. It is clear that the accuracy of the numerical results has been substantially improved by the new algorithm, which is robust when ΔT_{PC} is as small as 0.02°C. Use of the Lemmon formula is found to give somewhat better results, consistent with conclusions in previous work using linear interpolation.

Finally, for completeness, we note one or two points to do with the comparisons that have been made between numerical and theoretical results. The problem solved numerically is, of course, more or less different from that solved semi-analytically, in that the phase change is spread over a finite temperature interval. Although this may affect point values, its influence on average differences between the two solutions is likely to be small, and this seems to be confirmed by the rather weak dependence of $\bar{e}$ on ΔT_{PC} shown in *Figure 6*. The form of this dependence, though, is a little complicated and is believed to result from the interaction of errors resulting from the use of a finite ΔT_{PC}, with those due to discretization and linearization of the θ-method. These details leave unaffected our conclusion that the new algorithm provides an efficient and reliable way to handle latent heat using isoparametric biquadratic elements.

CONCLUSION

Methods that use spatial gradients of enthalpy to evaluate the effective specific heat, taking into account latent heat in phase change problems, have been shown to be prone to error if used in a straightforward way with quadratic interpolation of enthalpy. A modified procedure, using bilinear enthalpy sub-elements, formed by subdivision of the biquadratic temperature elements, is shown in our test problem to be accurate and robust, for phase change intervals ranging from 0.02 to 30°C.

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