An enriched finite element algorithm for the implicit simulation of the Stefan problem

Un algorithme d'éléments finis enrichis pour la simulation implicite du problème de Stefan

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ARTICLE INFO

ABSTRACT

An implicit enriched finite element algorithm is proposed to simulate heat transfer involving isothermal phase changes. This technique is based on a mixed variational formulation discretized by means of an enriched finite element approximation of the enthalpy in space. The interface is implicitly described without coupling with an interface-capturing technique. The time integration is carried out with an implicit (backward) Euler algorithm in time. Two examples in 1D and 2D clearly evidence the efficiency of the method developed.

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RÉSUMÉ

Un algorithme implicite de type éléments finis enrichis est proposé pour simuler des transferts de chaleur avec des changements de phase isothermes. Cette technique repose sur une formulation variationnelle mixte, discrétisée au moyen d'une approximation de l'enthalpie par éléments finis enrichis. L'interface est décrite de manière implicite sans couplage avec une technique spécifique de capture d'interface. L'intégration temporelle est réalisée par un algorithme d'Euler purement implicite en temps. Deux exemples 1D et 2D mettent clairement en évidence l'efficacité de la méthode développée.

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1. Introduction

Finite element analysis of heat transfer involving phase changes in solids is a numerical problem which has been extensively studied in the past years. It is well-known that the finite element simulation of such phenomena is confronted with computational pathologies when high latent heat effects appear such as, for example, during an isothermal transformation. One of the most famous solution method is the fixed grid technique well described in [1] and [2]. In this way, the latent heat effect can be easily overcome with an equivalent heat capacity [3–5]. The application of this technique raises problems since the phase change is spread over a small range of temperatures. One may easily numerically miss the very high (virtually infinite) peak of heat capacity, thus failing to respect exact conservation of energy.

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To overcome these difficulties, a mixed formulation has been introduced by Feulvarch et al. for the modeling of phase changes which can be isothermal, anisothermal, instantaneous or non-instantaneous [6]. The proposed formulation is based on the classical heat equation coupled with a function providing the temperature in terms of enthalpy. This enthalpy–temperature relation characterizes the kinetics of phase transformation and it includes the latent heat. Unfortunately, the FEM technique developed considers a continuous approximation of the temperature and the enthalpy which is not able to catch the jumps in the heat flux and in the enthalpy for isothermal phase changes.

The aim of this work is to improve this approach with a discontinuous finite element approximation of the enthalpy in space. It requires two fields which are the temperature and the enthalpy, while the method proposed by Chessa et al. [7] requires only one physical field which is the temperature. However, the technique of Chessa et al. requires a second auxiliary field which is a level set field needed to define the geometry of the interface of transformation. Its time evolution is carried out with an advection equation coupled with a forward-Euler algorithm. This severely limits the stability of the time integration: the authors propose to reset the level set field every two time steps.

The advantages of the method developed in this paper are three-fold:

- its enrichment functions which introduce a discontinuity on the enthalpy throughout the interface of phase change;
- its implicit geometry description of the interface which does not need any interface updating procedure (as for usual X-FEM applications);
- its implicit time integration based on the backward-Euler scheme ensuring good numerical stability without any restriction on the time step.

The paper is organized as follows. Section 2 is devoted to the general formulation of the problems envisaged and the enriched numerical scheme proposed. The solution procedure based on the iterative technique of Newton–Raphson is also presented. The examples proposed in Section 3 clearly show the potential and the efficiency of the method proposed.

2. Theory

2.1. Strong formulation

The problem studied in this paper is based on the formulation proposed by Feulvarch and Bergheau [6]:
Find functions T, H defined on $\Omega \times [0, T]$ verifying the initial–boundary value problem defined by

$$\begin{cases} \dot{H} = \mathrm{div}(\lambda \overrightarrow{\mathrm{grad}}\, T) & \text{in } \Omega \\ T = g(H) & \text{in } \Omega \\ \lambda \overrightarrow{\mathrm{grad}}\, T \cdot \vec{n} = q^{(p)} + k(T^{(p)} - T) & \text{on } \partial\Omega \end{cases} \tag{1}$$

with the initial condition

$$H(t=0) = H_0$$

In these equations, λ is the thermal conductivity which can be temperature-dependent; g is the function providing the temperature in terms of the enthalpy[1]; $\vec{n}$ is the unit outward normal vector to the boundary; $q^{(p)}$ is a prescribed "input flux"; $T^{(p)}$ is a prescribed value of the temperature and k is a "transfer coefficient". As is well-known, the general boundary conditions $(1)_3$ encompass both the cases of a prescribed flux (for $k = 0$) and a prescribed value of T (for $k \to +\infty$).

It is worth noting that the partial differential equation (1) implies continuity of the function T, but *not* of the function H. Indeed, in the case of an isothermal transformation, the enthalpy H can be expressed as the sum of continuous function h and a discontinuous one providing the enthalpy of transformation ΔH due to the phase change:

$$H = h + \mathcal{I}_d \Delta H$$

where $\mathcal{I}_d$ is a function which indicates the state of the transformation:

$$\mathcal{I}_d = \begin{cases} 1 & \text{if the transformation occurred} \\ 0 & \text{otherwise} \end{cases}$$

2.2. Weak formulation

The weak formulation of the problem is classically obtained by multiplying equation $(1)_1$ by a weighting function T^*, Eq. $(1)_2$ by a weighting function H^*, and integrating over the domain Ω. Integrating the first equation by parts and accounting for the boundary condition $(1)_3$, one thus obtains the following variational formulation of the problem:

---

[1] Eq. $(1)_2$ cannot be inverted to yield the temperature T as a function of the enthalpy H in the case of an isothermal transformation.

Find functions T, H such as for all functions T*, H*,

$$
\begin{cases}
\displaystyle\int_\Omega \dot{H}T^* \,\mathrm{d}V + \int_\Omega \lambda \overrightarrow{\mathrm{grad}}\, T \cdot \overrightarrow{\mathrm{grad}}\, T^* \,\mathrm{d}V + \int_{\partial\Omega} kTT^* \,\mathrm{d}S - \int_{\partial\Omega} (q^{(p)} + kT^{(p)})T^* \,\mathrm{d}S = 0 \\
\displaystyle\int_\Omega [T - g(H)]H^* \,\mathrm{d}V = 0
\end{cases}
\tag{2}
$$

2.3. Time discretization

An implicit (backward) Euler algorithm tolerating relatively large time steps is adopted for the time integration:

$$
\dot{H}(t + \Delta t) \simeq \frac{H(t + \Delta t) - H(t)}{\Delta t}
$$

The variational formulation (2), written at time $t + \Delta t$, then becomes:

Find functions $T_{t+\Delta t}$, $H_{t+\Delta t}$ such as for all functions T*, H*,

$$
\begin{cases}
\displaystyle\int_\Omega \frac{H_{t+\Delta t} - H_t}{\Delta t} T^* \,\mathrm{d}V + \int_\Omega \lambda \overrightarrow{\mathrm{grad}}\, T_{t+\Delta t} \cdot \overrightarrow{\mathrm{grad}}\, T^* \,\mathrm{d}V + \int_{\partial\Omega} kT_{t+\Delta t}T^* \,\mathrm{d}S - \int_{\partial\Omega} (q^{(p)} + kT^{(p)})T^* \,\mathrm{d}S = 0 \\
\displaystyle\int_\Omega [T_{t+\Delta t} - g(H_{t+\Delta t})]H^* \,\mathrm{d}V = 0
\end{cases}
\tag{3}
$$

2.4. Spatial discretization

Following the usual procedure, the discretization of the temperature T is of the form

$$
T(\vec{x}) = \sum_{i=1}^{N} T_i N_i(\vec{x})
\tag{4}
$$

In this expression, N denotes the number of nodes, T_i is the value of the function T at node i and $N_i(\vec{x})$ is the shape function associated to this node.[2] One can note that this classical finite element approximation smooths naturally the discontinuity of the heat flux throughout the interface of transformation. As far as the enthalpy approximation is concerned, a discontinuous finite element approximation is proposed as follows:

$$
H(\vec{x}) \approx H^{disc}(\vec{x}) = \sum_{i=1}^{N} h_i N_i(\vec{x}) + \mathcal{I}_d \Delta H
\tag{5}
$$

Following Galerkin's standard approach, the test functions T^* and H^* are taken in the same form than T and h. Let $\{\mathbf{T}\} \equiv (T_i)_{1 \leqslant i \leqslant N}$, $\{\mathbf{h}\} \equiv (h_i)_{1 \leqslant i \leqslant N}$ denote the vectors of nodal values of the functions T and h. Substituting the nodal approximations (4)–(5) into the variational formulation (3), one obtains the following non-linear system of equations:

$$
\begin{cases}
\{\mathbf{R_T}\} \equiv [\mathbf{K}].\{\mathbf{T}(t + \Delta t)\} + [\mathbf{M}] \cdot \dfrac{\{\mathbf{h}(t + \Delta t)\} - \{\mathbf{h}(t)\}}{\Delta t} + \dfrac{\{\mathbf{Q}(t + \Delta t)\} - \{\mathbf{Q}(t)\}}{\Delta t} - \{\mathbf{F}\} = \{\mathbf{0}\} \\
\{\mathbf{R_h}\} \equiv [\mathbf{M}] \cdot \{\mathbf{T}(t + \Delta t)\} - \{\mathbf{G}(t + \Delta t)\} = \{\mathbf{0}\}
\end{cases}
\tag{6}
$$

In this system $[\mathbf{K}] \equiv (K_{i,j})_{1 \leqslant i,j \leqslant N}$ and $[\mathbf{M}] \equiv (M_{i,j})_{1 \leqslant i,j \leqslant N}$ are "stiffness" and "mass" matrices defined by

$$
\begin{cases}
\displaystyle K_{i,j} \equiv \int_\Omega \lambda \overrightarrow{\mathrm{grad}}\, N_i \cdot \overrightarrow{\mathrm{grad}}\, N_j \,\mathrm{d}V + \int_{\partial\Omega} kN_i N_j \,\mathrm{d}S \\
\displaystyle M_{i,j} \equiv \int_\Omega N_i N_j \,\mathrm{d}V
\end{cases}
\tag{7}
$$

and $\{\mathbf{Q}\} \equiv (Q_i)_{1 \leqslant i \leqslant N}$, $\{\mathbf{F}\} \equiv (F_i)_{1 \leqslant i \leqslant N}$ and $\{\mathbf{G}\} \equiv (G_i)_{1 \leqslant i \leqslant N}$ are vectors defined by

---

[2] N_i^e denoting the shape function associated to node i in element e, $N_i(\vec{x})$ is defined as the common value of the quantities $N_i^e(\vec{x})$ where e varies among the elements containing $\vec{x}$.

$$\begin{cases} Q_i \equiv \displaystyle\int_{\Omega} \mathcal{I}_d \Delta H N_i \, dV \\[4mm] F_i \equiv \displaystyle\int_{\partial\Omega} \left(q^{(p)} + kT^{(p)}\right) N_i \, dS \\[4mm] G_i \equiv \displaystyle\int_{\Omega} g\!\left(H^{disc}\right) N_i \, dV \end{cases} \tag{8}$$

2.5. Solution procedure

The resolution of system (6) at each instant seems very difficult by means of a classical Newton–Raphson or any equivalent iterative method. Indeed, the derivative of the function $\mathcal{I}_d$ is equal to zero. Therefore, the influence of the temperature or the enthalpy on the interface position is not taken into account in the tangent stiffness matrix needed for the application of the Newton–Raphson technique. Experiences show that this leads to high difficulties to achieve convergence. Moreover, the convergence depends very clearly on the numerical integration scheme implemented for the computation of Q_i. To avoid this difficulty, a continuous finite element approximation is introduced for the enthalpy:

$$H(\vec{x}) \approx H^{cont}(\vec{x}) = \sum_{i=1}^{N} H_i \, N_i(\vec{x}) \tag{9}$$

This approximation H^{cont} is taken equal to the discontinuous approximation H^{disc} in a weak sense at each time step:

$$\forall \delta H^{cont}, \quad \int_{\Omega} \delta H^{cont}\!\left(H^{cont} - H^{disc}\right) dv = 0 \quad \Longrightarrow \quad [\mathbf{M}] \cdot \{\mathbf{H}\} = [\mathbf{M}] \cdot \{\mathbf{h}\} + \{\mathbf{Q}\} \tag{10}$$

where $\{\mathbf{H}\} \equiv (H_i)_{1 \leqslant i \leqslant N}$ denote the vector of nodal values of the function H approximated by (9).

From this change of variable, system (6) becomes

$$\begin{cases} \{\mathbf{R_T}\} \equiv [\mathbf{K}] \cdot \{\mathbf{T}(t + \Delta t)\} + [\mathbf{M}] \cdot \dfrac{\{\mathbf{H}(t + \Delta t)\} - \{\mathbf{H}(t)\}}{\Delta t} - \{\mathbf{F}\} = \{\mathbf{0}\} \\[4mm] \{\mathbf{R_h}\} \equiv [\mathbf{M}] \cdot \{\mathbf{T}(t + \Delta t)\} - \{\mathbf{G}(t + \Delta t)\} = \{\mathbf{0}\} \end{cases} \tag{11}$$

Eqs. (11) are solved by a Newton–Raphson iterative method. The tangent matrix to be used in this method is

$$\begin{bmatrix} \dfrac{\partial \{\mathbf{R_T}\}}{\partial \{\mathbf{T}(t + \Delta t)\}} & \dfrac{\partial \{\mathbf{R_T}\}}{\partial \{\mathbf{H}(t + \Delta t)\}} \\[3mm] \dfrac{\partial \{\mathbf{R_h}\}}{\partial \{\mathbf{T}(t + \Delta t)\}} & \dfrac{\partial \{\mathbf{R_h}\}}{\partial \{\mathbf{H}(t + \Delta t)\}} \end{bmatrix} = \begin{bmatrix} [\mathbf{K}] & \dfrac{[\mathbf{M}]}{\Delta t} \\[3mm] [\mathbf{M}] & -[\mathbf{L}] \end{bmatrix} \tag{12}$$

In this equation $[\mathbf{L}] \equiv (L_{i,j})_{1 \leqslant i,j \leqslant N}$ is the matrix defined (at each iteration) by

$$L_{i,j} \approx \int_{\Omega} \frac{\partial g}{\partial H}\!\left(\{\mathbf{H}(t + \Delta t)\}\right) N_i N_j \, dV \tag{13}$$

One can note that this approximation is introduced only in the matrix $[\mathbf{L}]$, not in the vector $\{\mathbf{R_h}\}$, so it has no effect upon the "exactness" of the numerical solution. Each iteration thus consists of solving a linear system to compute the increments $\{\delta\mathbf{T}\}$ and $\{\delta\mathbf{H}\}$ of $\{\mathbf{T}(t + \Delta t)\}$ and $\{\mathbf{H}(t + \Delta t)\}$:

$$\begin{bmatrix} [\mathbf{K}] & \dfrac{[\mathbf{M}]}{\Delta t} \\[3mm] [\mathbf{M}] & -[\mathbf{L}] \end{bmatrix} \cdot \begin{Bmatrix} \{\delta\mathbf{T}\} \\[2mm] \{\delta\mathbf{H}\} \end{Bmatrix} = - \begin{Bmatrix} \{\mathbf{R_T}\} \\[2mm] \{\mathbf{R_h}\} \end{Bmatrix} \tag{14}$$

and computing the vector $\{\mathbf{h}(t + \Delta t)\}$ from (10). The function $\mathcal{I}_d$ needed for the computation of $\{\mathbf{Q}\}$ in (10) can be defined by an Heaviside function which can depend on the temperature or the enthalpy. Experiences show that the enthalpy leads to a better stability of the solution. Therefore, $\mathcal{I}_d$ is defined by the Heaviside function as follows:

$$\mathcal{I}_d = \mathcal{H}\!\left(H^{cont} - H_m\right) = \begin{cases} 1 & \text{if } H^{cont} - H_m > 0 \\ 0 & \text{otherwise} \end{cases} \tag{15}$$

where H_m denotes the intermediate value of the enthalpy during the transformation. Contrary to the classical X-FEM applications [7–9], this formulation integrates implicitly the interface position by means of the field H^{cont} which is an unknown of the physical problem.
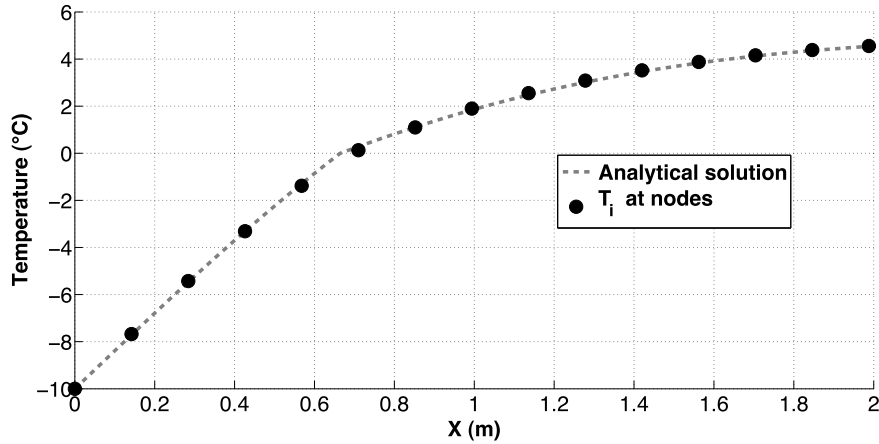
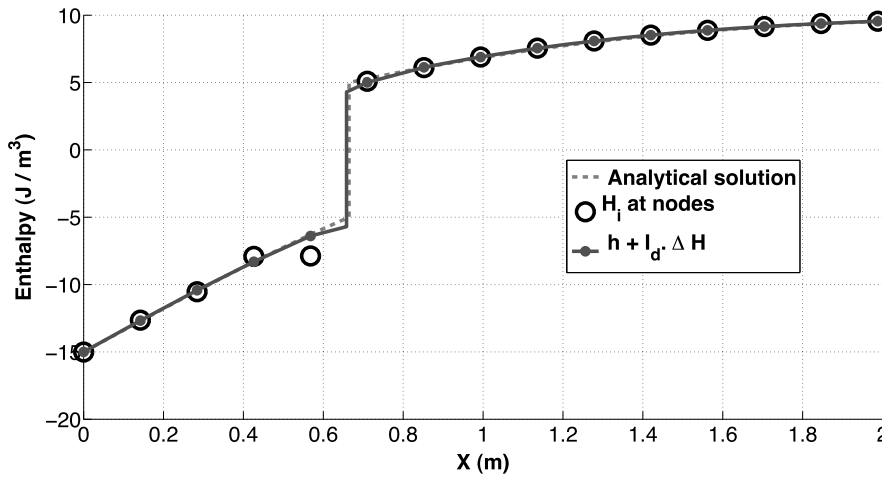**Fig. 1.** Temperature distributions at time $t = 0.5$ s.

Fig. 2. Enthalpy distributions at time $t = 0.5$ s.

3. Application to the Stefan problem

A test is performed on Stefan's famous problem of isothermal solidification of an initially liquid semi-infinite slab. The values of the thermal conductivity and the enthalpy of transformation are respectively taken equal to 1 W m^{-1} K^{-1} and 10 J m^{-3}. In this example the derivative dg/dH of the temperature with respect to the enthalpy per unit volume is strictly zero during the transformation and equal to 1 elsewhere. The initial temperature of 5 °C is bigger than the temperature of transformation equal to 0 °C.

The finite element mesh is composed of linear elements. The element size Δx is uniform and the time step Δt is invariable ($\Delta x = 0.142$ m, $\Delta t = 0.01$ s). The results are obtained with less than 5 iterations per time step with the Newton–Raphson method. Figs. 1 and 2 show the computed temperature and enthalpy distributions at time $t = 0.5$ s, together with those corresponding to the analytical solution given in [10]. Fig. 3 also presents the evolution of the position x_f of the interface in time defined by $H^{cont} = H_m$ as proposed in (15). The numerical results closely agree with the analytical evolution even if oscillations are shown in Fig. 3. They certainly come from the fact that the discontinuity of the temperature gradient is not taken into account.

To show the capability of the method developed for multi-dimensional problems, the same problem is considered, but now near a square corner of 1 m side ($\Delta x = 0.142$ m, $\Delta t = 0.01$ s) with an initial temperature of 25 °C. Fig. 4 shows the mesh composed of 49 bilinear elements and the distributions of temperature and enthalpy at time $t = 0.3$ s. These results have been obtained with less than 5 iterations per time step.

4. Conclusion

An implicit technique has been proposed to simulate heat transfer involving isothermal phase changes. This technique is based on a mixed variational formulation discretized by means of an enriched finite element approximation of the enthalpy
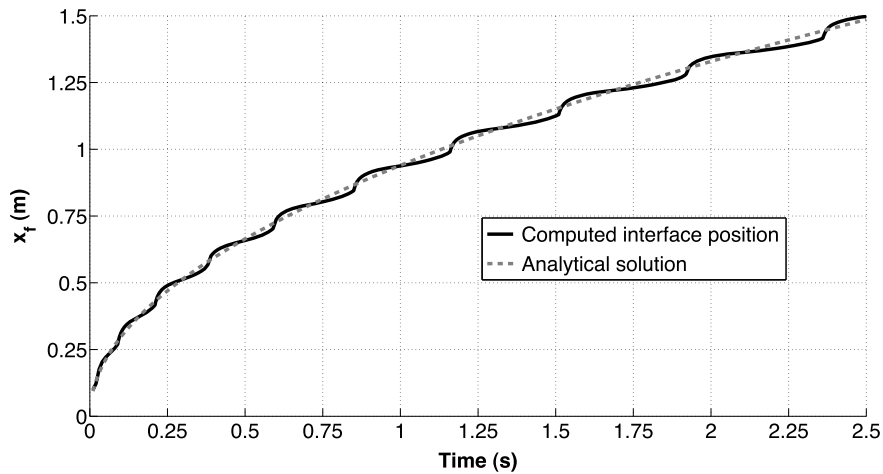
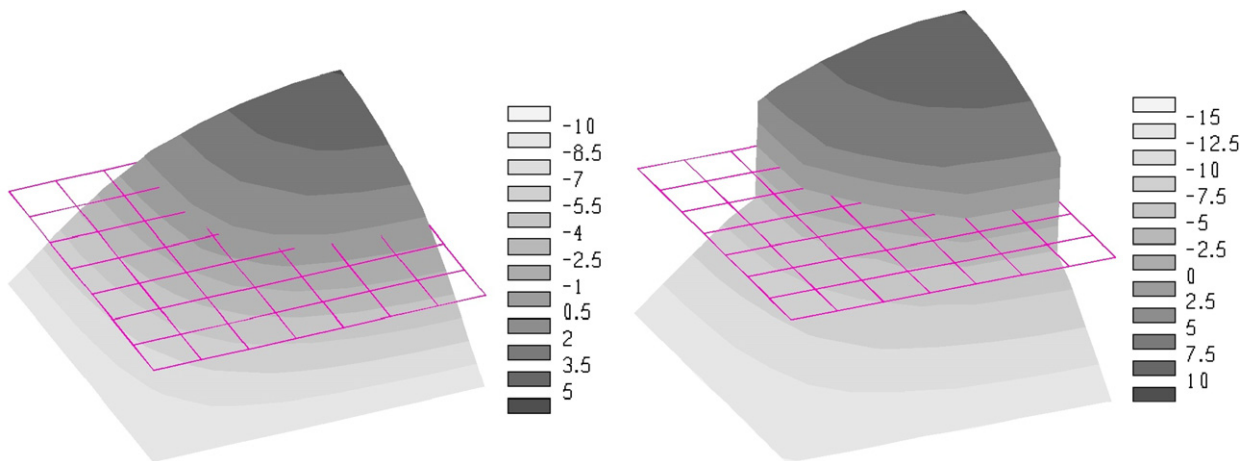**Fig. 3.** Evolution of the phase change interface in time.

Fig. 4. Temperature (°C) and enthalpy (J/m^3) distributions at time $t = 0.3$ s.

in space. The interface is implicitly described by a continuous approximation of the enthalpy which plays the role of a level set to represent the geometry of the transformation interface. The time integration is carried out with an implicit (backward) Euler algorithm in time tolerating large time step for the computation. Two examples in 1D and 2D clearly evidence the efficiency of the method developed.

References

[1] V.R. Voller, An overview of numerical methods for phase change problems, Advances in Numerical Heat Transfer 1 (1996) 341–375.
[2] E. Feulvarch, J.M. Bergheau, J.B. Leblond, An implicit finite element algorithm for the simulation of diffusion with phase changes in solids, International Journal for Numerical Methods in Engineering 78 (2009) 1492–1512.
[3] G. Comini, S. Del Guidice, R.W. Lewis, O.C. Zienkiewicz, Finite element solution of nonlinear heat conduction problems with special reference to phase change, International Journal for Numerical Methods in Engineering 8 (1974) 613–624.
[4] K. Morgan, R.W. Lewis, O.C. Zienkiewicz, An improved algorithm for heat conduction problems with phase change, International Journal for Numerical Methods in Engineering 12 (1978) 1191–1195.
[5] R. Lewis, P. Roberts, Finite element simulation of solidification problems, Applied Scientific Research 44 (1987) 61–92.
[6] E. Feulvarch, J.M. Bergheau, An implicit fixed-grid method for the finite-element analysis of heat transfer involving phase changes, Numerical Heat Transfer, Part B: Fundamentals 51 (2007) 585–610.
[7] J. Chessa, P. Smolinski, T. Belytschko, The extended finite element method for solidification problems, International Journal for Numerical Methods in Engineering 53 (2002) 1959–1977.
[8] R. Merle, J. Dolbow, Solving thermal and phase change problems with the extended finite element method, Computational Mechanics 28 (2002) 339–350.
[9] H. Ji, D. Chopp, J.E. Dolbow, A hybrid extended finite element/level set method for modeling phase transformations, International Journal for Numerical Methods in Engineering 54 (2002) 1209–1233.
[10] H. Carslaw, J. Jaeger, Conduction of Heat in Solids, Clarendon Press, Oxford, UK, 1959.